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A correlation of the idealized heat of vaporization to molecular weight

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A CORRELATION OF THE IDEALIZED HEAT OF VAPORIZATION TO MOLECULAR WEIGHT

BY

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I. INTRODUCTION

Using the Clausius-Clapeyron equation[18] as a base,

$$\log P = \frac{-\Delta H}{2.303R}\frac{1}{T} + C \qquad (1)$$

many investigators have tried to develop variations to better describe both ideal and non-ideal systems. The literature is abundant with correlations of vapor pressure to temperature and associated correlations of latent heats of vaporization to molecular characteristics; often molecular weight or carbon number.

In studying various approaches to these correlations, Ibrahim and Kuloor[16] have observed that; "In general, correlations that are purely theoretical are not successful, whereas those that are semi-empirical can predict pure compor latent heats of vaporization with a surprisingly good degree of accuracy."

Van Ness[40], in his presentation to the Applied Thermodynamic Symposium in 1967, reinforced the role of empiricism when he stated that "... at present no generally satisfactory theory exists that provides a sound basis for either the prediction or correlation of thermodynamic data for binary liquid mixtures. Until such a theory appears, the incentive remains to develop empirical methods to their ultimate refinement."

With this in mind, many interesting examples of correlations can be found for vapor-liquid equilibrium data and latent heat of vaporization data.

Beginning with the boiling point as a variable, one of the most familiar correlations is Troutons rule:

$$\frac{\Delta H_v}{\text{Boiling Point}(^oK)} = 21 \text{ cal./mole/degree} \quad (2)$$

Hildebrand[13,8] offered an improvement on this when he observed that for unassociated liquids, the entropies of vaporization are equal at the temperature at which their vapors occupy equal volumes. When a vapor concentration of 0.005 mole/liter is used, the constant is 27.

Anderson[1] has found the Kinney equation:

$$\text{B.P.}(^oC) = 230.14(\text{total boiling point number})^{1/3} - 543 \quad (3)$$

well suited to calculating the boiling points of perfluoroalkanes. The boiling point number is calculated from contributions based on molecular structure.

For n-paraffins, Tettramanti and co-workers[39] have found a linear relationship between molecular weight and boiling point.

$$\frac{\Delta\text{Molecular Weight}}{\Delta\text{Boiling Point}} = 1.2471 \times 10^{-1} + 3.02008 \times 10^{-3} \text{ Ma} \quad (4)$$

where Ma is the average molecular weight over the interval.

Several direct variations on the Clausius-Clapeyron equation form have also been presented.

A popular variation is the Antoine equation:

$$\log P \qquad B \qquad (5)$$

Nakanishi[25] has related the coefficients of this equation to the carbon numbers (n) of n-paraffins by expanding them as power series of (n - 4). A is expanded to the third order while B and C are expanded to the second order. The coefficients reported for the expansions are:

a_o = 6.83029 a_1 = 0.015108 a_2 = 0.007777 a_3 = -0.001482

b_o = 945.90 b_1 = 123.985 b_2 =-5.467

c_o = 240.00 c_1 = -8.0983 c_2 = 0.1255

This investigator also presents a technique for calculating an effective carbon number and therefor extends his equation to non-paraffins.

Frost and Kalkwarf[10] have developed the following relationship:

$$\log P = A + \frac{B}{T} + C \log T + D \frac{P}{T^2} \qquad (6)$$

Thodos and co-workers[3,33,36,37] have devoted a great deal of study to this equation and have found it to accurately predict vapor pressures from the triple point to the critical point for saturated and unsaturated aliphatic, aromatic, and naphthenic hydrocarbons.

Correlations of one or more of the constants to molecular weight or carbon number are presented for each of the classes but there is no common correlation for the entire group of compounds.

Narsimhan[28] has used the Clausius-Clapeyron equation in reduced form to generate an expression which has been found

to accurately predict the vapor pressure of both polar and non-polar liquids.

$$-\ln P_r = \beta f(T_r) \tag{7}$$

where $$\beta = \frac{0.1127 \ln P_c}{(0.80 - T_{rb})}$$

$$f(T_r) = -(\ln T_r - .b(1/T_r - 1) - \frac{b^2}{4}(1/T_r^2 - 1) - \frac{b^3}{18}(1/T^3 - 1) \ldots)$$

and $b = 0.8832$.

A review of correlations involving heat of vaporization directly yields an even more abundant list of examples. Among the well established relationships are:

The Haggenmacher[18] equation:

$$\Delta H_v = \frac{4.576\ BT^2(1 - P_r/T_r^3)^{0.5}}{(T + C)^2} \tag{8}$$

B and C are Antoine Constants.

The Kistiakowsky-Fishtine equation[8]:

$$\frac{\Delta H_{vb}}{T_b} = K_k(8.75 + 4.576 \log T_b) \tag{9}$$

where K_k is a constant dependent on carbon number and type of motecule.

The Pitzer equation[8]:

$$\Delta H_v = T(\Delta S_v^o + \omega \Delta S_v') \tag{10}$$

where ΔS_v^o and $\Delta S_v'$ are tabulated according to reduced temperature and ω, the acentric factor, is dependent on the reduced pressure.

$\omega = -\log P_r - 1.000$

The Watson equation[8] which relates heat of vaporization at some reduced temperature to that at the reduced boiling point:

$$\Delta H_v = \Delta H_{vb} \left(\frac{1 - T_r}{1 - T_{rb}} \right)^{0.38} \qquad (11)$$

The Modified Othmer[8,9,31,32] Method, where a reference liquid, usually water, is used:

$$\Delta H_v = m \left(\frac{\Delta H_{vw} \Delta Z}{\Delta Z_w} \right)_T \qquad (12)$$

w indicates water. ΔZ the compressibility factor must be calculated or estimated from a table.

$m = \frac{d \ln P}{d \ln P_w}$

The latter expression may be written

$$\log P = m \log P_w + C \qquad (13)$$

and Othmer has related m and C to the carbon number (n) for a homologous series.

$$m = b' n^a \qquad (14)$$

$$C = An + B \qquad (15)$$

Values of the constants are given by Table 1.

TABLE 1

Constants for Othmer Equation

Series	Range	b'	a	A	B
Normal hydrocarbons	n = 5-17	0.1852	0.785	-0.352	2.51
Alcohols	n = 2-8	0.857	0.198	-0.344	1.042
Acids	n = 1-8	0.7105	0.411	-0.351	0.510

A modification of the Watson equation has been used by Narsimhan[26,27,29] and Bradford and Thodos[5] to develop the following correlations. In this equation a hypothetical heat of vaporization at $0^{o}K$ (ΔH_o) is defined and the Watson equation becomes:

$$\Delta H_v = \Delta H_o (1 - T_r)^{0.38} \qquad (16)$$

Using this expression of ΔH_v as a function of T_r, and the Clapeyron equation in reduced form, Narsimhan related ΔH_v to reduced variables alone.

$$\Delta H_v = \frac{1.987 T_c (\ln P_c)(1 - T_r)}{(1.963 - 2.46 T_{rb})} \qquad (17)$$

where $\Delta H_o = RT_c \ln P_c$.

Narsimhan also developed an expression for ΔH_o as a function of critical volume:

$$\Delta H_o = (\alpha a^{5/4} K^{3/8} V_c^{.42}) \qquad (18)$$

where α is a constant.

Herzog's constant, (a), is equal to 3.34 for compounds containing the functional groups -CO, -C≡N, -COOH, and -OH;

and 2.92 for all others.

K is the constant for the Katayama modification of Eotvo's equation:

$$K = \frac{-1}{T_r} \frac{d}{dT_r} \left[\sigma \left(\frac{M}{d_l - d_v} \right)^{2/3} \right]$$

d = density

σ = surface tension

M = molecular weight

Bradford and Thodos determined the coefficients of the Frost and Kalkwarf equation (6) for a large number of hydrocarbons, calculated ΔH_v, and plotting log ΔH_v vs. log$(1-T_r)$ successfully generated the Watson equation (16) with an exponent of 0.39.

They further demonstrated that, for hydrocarbons:

$$\Delta H_o = 800\ M^{0.72} \qquad (19)$$

Kuloor and co-workers[16,41] have developed relationships of ΔH_v at the boiling point both to reduced variables and to molecular weight.

$$\Delta H_{vb} = \frac{4.7 T_c\ (1 - P_{rb})^{0.69} \log P_{rb}}{(1 - 1/T_{rb})} \qquad (20)$$

and

$$\Delta H_{vb} = \frac{C}{M^n} \quad \text{(cal/g)} \qquad (21)$$

where the constants C and n are determined for each homologous series. (Table 2)

TABLE 2

Constants for Kuloor Equation

Homologous Series	C	n
Ethers	315	0.300
Esters	1550	0.642
Acids	7200	0.936
Ketones	3200	0.795
Aldehydes, oxides, anhydrides	940	0.494
Aromatics	1155	0.574
Aliphatics	367	0.342
Alcohols	3475	0.745
Cyclic hydrocarbons	605	0.440
Substituted aliphatics	1280	0.650
Amines	3250	0.825
Nitrogen compounds	2160	0.690

In his study of normal paraffins, Nagata[24] related heat of vaporization to carbon number.

$$\log (\Delta H_{vn} - \Delta H_{vK}) = 4.9331 - 2.2189\ n^{0.33} \quad (22)$$

Unfortunately his definition of ΔH_{vK} is not clear.

Other correlations involving reduced variables have been developed by Bondi and Simkin[4], Chen[6], Graue, Berry, and Sage[11], and Kunte and Doraiswamy[19], but they are quite similar to approaches which have already been discussed and no attempts were made to involve molecular properties.

Correlations to other molecular properties include:

Desai's[7] correlation to density;

$$\Delta H_v = K(D - d)^{7/5} \quad (23)$$

D = liquid density

d = vapor density

K = constant

and Wright's[42] similar work which involves molecular

weight;

$$\Delta H_v^{(.8)} \cong \frac{[L](D - d)}{M} \qquad (24)$$

where L has been tabulated for many compounds.

Lastly, Ogden and Lielmezs[30] related ΔH_v at the boiling point to Altenburg's Quadratic Mean Radius:

$$\Delta H_{vb} = q\, X^b \qquad (25)$$

where

$$X = \overline{R_v^2} / a_i^2$$

a_i^2 = distance between molecules

R_v^2 = quadratic mean radius

q and b are constants.

Using the published values for R_v^2 and a_i^2, the authors determined the following values for q and b which are given in Table 3.

TABLE 3

Ogden-Lielmezs Equation Constants

Homologous Series	q	b
n-alkanes	5.935	0.467
Cyclic alkanes	7.158	0.279
Benzenes	7.801	0.261
Alkane isomers	6.331	0.489

From the examples which have been cited, it is obvious that many correlations exist which accurately predict heats of vaporization and describe P-T behavior under specific

circumstances. However, a shortcoming of many of these correlations is their limited application to only certain classes of compounds.

All of the equations suffer from one or more of the following restrictions:

- apply to a limited class of compounds which demonstrate near ideal behavior (hydrocarbons).

- if applicable to a wider range of compounds, require unique constants for each homologous series which bear no relation to the homologous series.

- require prior knowledge of specific molecular properties which may not be readily available or calculable (T_c, P_c, D, d, ... etc.)

- are too complex to be easily handled.

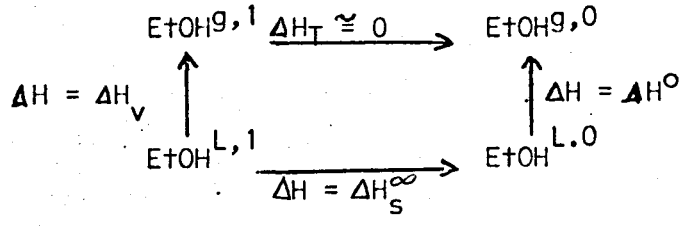
Preston and Prausnitz[43] published a method for determining Henry's law constants from a reduced empirical equation of state which accurately predicts the variation of Henry's law constant with temperature for the substances studied. Unfortunately, this work was published too late to be considered in our work.

II. OBJECTIVE

In an attempt to develop a simplified and more generally applicable correlation of heat of vaporization, a new term, idealized heat of vaporization (ΔH^{o}), is defined.

The idealized heat of vaporization is calculated from the Clausius-Clapeyron equation (1) using vapor pressures which reflect the behavior of the molecule in question in the infinitely dilute state in a non-polar solvent.

To put ΔH^{o} into perspective with the regular heat of vaporization (ΔH), consider the following schematic for the vaporization of ethanol (EtOH).



where g - gas

L - liquid

1 - pure state

0 - infinite dilution for solutes or zero pressure for gases

ΔH_S^{∞} - heat of dilution from the pure to the infinitely dilute state

ΔH_T - JOULE THOMSON DH

We see here that

$$\Delta H^{o} = (\Delta H_V - \Delta H_S^{\infty})$$

This will be discussed in more detail in Section V.

The object of this thesis is to develop the necessary procedures to calculate the idealized heat of vaporization,

(ΔH^{o}), express its correlation to molecular weight, (M), and compare this to a similar correlation for regular heats of vaporization.

To this end seventeen compounds of various molecular classes have been studied.

III. METHOD

We will determine ΔH^o by applying the Clausius-Clapeyron equation to the infinitely dilute solute. Consider Figure 1, a typical plot of solute vapor pressure versus solute mole fraction.

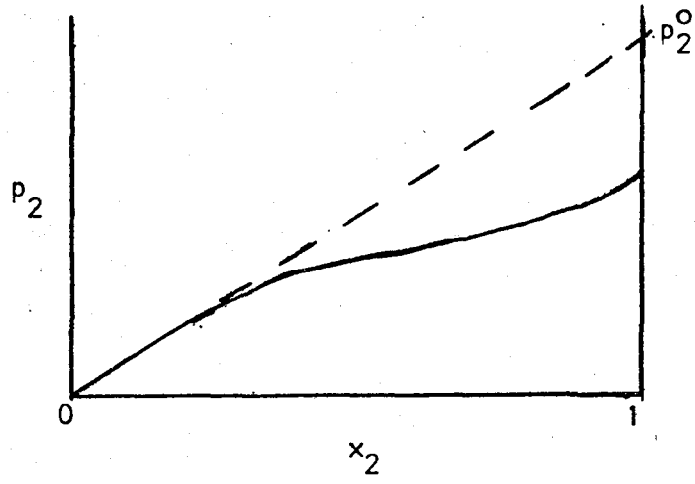


FIGURE 1

Henry's law, which is obeyed by the infinitely dilute solution is

$$p_2 = k_H x_2 \tag{27}$$

At $x_2 = 1$, $p_2 = p_2^o$ and $p_2^o = k_H$. Thus k_H can be interpreted as the vapor pressure the solute would have if, when pure, its molecules had the same liquid state environment as in the infinitely dilute solution. Application of the Clausius-Clapeyron equation to p_2^o gives the desired ΔH^o

$$\frac{d \ln p_2^o}{dT} = \frac{\Delta H^o}{RT^2} \tag{28}$$

This will be explained in more detail later.

Curve Fitting

To determine the partial pressure of a molecule in the infinitely dilute state in a non polar solvent, (p_2^o), it is

necessary to determine the relationship between partial pressure of the solute and the mole fraction of the solute in the liquid, $p_2 = f(x_{2l})$. The slope of this relationship at infinite dilution

$$\lim_{x_{2l} \to 0} \left(\frac{dp_2}{dx_{2l}} \right) = k_H = p_2^o \tag{29}$$

then gives the desired information.

Since no general relationship for $f(x_{2l})$ is available, an n^{th} order power series of x_{2l} has been used to estimate the function.

$$p_2 = a_o + a_1 x_{2l} + a_2 x_{2l}^2 + a_3 x_{2l}^3 \ldots\ldots a_n x_{2l}^n \tag{30}$$

Differentiating (29) gives

$$\frac{dp_2}{dx_{2l}} = a_1 + 2a_2 x_{2l} + 3a_3 x_{2l}^2 \ldots na_n x_{2l}^{n-1} \tag{31}$$

from which

$$\lim_{x_{2l} \to 0} \left(\frac{dp_2}{dx_{2l}} \right) = a_1 = k_H = p_2^o \tag{32}$$

Similar use of the polynomial power series has been sucessfully made by many investigators[21,23,38]

Li[20] has shown that the application of any available boundary conditions during the power series determination greatly increases the accuracy of the overall function $\left(\sum_n^n a_i x_{2l}^n \right)$.

In this case, an initial boundary condition is known;

the partial pressure of the solute, (p_2), is necessarily zero when its mole fraction in the solvent, (x_{21}), is zero. The function $p_2 = f(x_{21})$ must therefore pass through the origin.

The general form for the power series is given by (33)

$$p_2 = \sum_{n=0}^{n} (a_n x_{21}^{\ n}) = a_o + a_1 x_{21} + a_2 x_{21}^{\ 2} + \dots a_n x_{21}^{\ n}$$

Applying the boundary condition, (33) becomes

$$p_2 = \sum_{n=1}^{n} (a_n x_{21}^{\ n}) = a_1 x_{21} + a_2 x_{21}^{\ 2} + a_3 x_{21}^{\ 3} \dots a_n x_{21}^{\ n} \quad (34)$$

The coefficients of the power series were calculated using the principle of least squares:

For illustration, consider a power series similar to (29).

In general terms

$$y_i = f(x_i) = \sum_{n=1}^{n} a_n x^n \quad (35)$$

where $i = i^{th}$ point pair.

The error, ($\mathcal{E}_i$), in y_i is the difference between the calculated value and the observed value.

$$\mathcal{E}_i = f(x_i) - y_i \quad (36)$$

The square of this error is:

$$\mathcal{E}_i^2 = f^2(x_i) - 2y_i f(x_i) + y_i^2 \quad (37)$$

This may be calculated for each observed point and summed.

$$\sum_i \mathcal{E}_i^2 = \sum_i f^2(x_i) - 2\sum_i y_i \left[f(x_i)\right] + \sum_i y_i^2 \quad (38)$$

The principle of least squares states that the best fit to the locus of points is obtained when $\sum_i \mathcal{E}_i^2$ is minimized.

The partial derivative of (38) with respect to each of the unknown coefficients, (a_n), is thereby determined and set equal to zero.

$$\frac{\partial \sum_i \varepsilon_i^2}{\partial a_n} = 0 \Bigg|_{n=1}^{n} \tag{39}$$

This group of equations may then be solved simultaneously to give the values of each a_n.

Using matrix notation, these calculations can be simplified:

Let

$$Y = \begin{bmatrix} y_1 \\ y_2 \\ \cdot \\ \cdot \\ \cdot \\ y_i \end{bmatrix}$$

$$X = \begin{bmatrix} x_1 & x_1^2 & x_1^3 & \cdots & x_1^m \\ x_2 & x_2^2 & x_2^3 & \cdots & x_2^m \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdot & \cdots & \cdot \\ x_i & x_i^2 & x_i^3 & \cdots & x_i^m \end{bmatrix}$$

$$X' = \text{transpose of } X = \begin{bmatrix} x_1 & x_2 & \cdots & x_i \\ x_1^2 & x_2^2 & \cdots & x_i^2 \\ x_1^3 & x_2^3 & \cdots & x_i^3 \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ \cdot & \cdot & \cdots & \cdot \\ x_1^m & x_2^m & \cdots & x_i^m \end{bmatrix}$$

$$A = \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ \cdot \\ \cdot \\ \cdot \\ a_m \end{bmatrix}$$

where m = maximum order of the power series.

The least squares solution becomes

$$A = (X'X)^{-1} X'Y \tag{40}$$

$(X'X)^{-1}$ is the inverse of $(X'X)$.

The variance in each coefficient may be found by calculating the matrix

$$S = \frac{[(Y'Y) - (A'X')Y]}{\text{degrees of freedom}} \tag{41}$$

$\sigma^2_{a_{ii}} = S \times$ [diagonal element of $(X'X)^{-1}$]

The diagonal elements of this matrix

$$S_{11}, S_{22}, S_{33}, \ldots S_{mm}$$

are each the variance of their respective coefficient a_1, a_2, a_3, ... a_m.

The standard error for each coefficient is the square root of its variance.

$$\sigma_{a_n} = \sqrt{S_{nn}} \tag{42}$$

The standard error of the total estimate is given by:

$$\sigma_{est} = \sqrt{\frac{\Sigma (y_{i\ Obs} - y_{i\ Calc})^2}{N}} \tag{43}$$

where N = number of points.

The Student's t test can be used to establish the confidence in each coefficient. In this case

$$t = \frac{a_n}{\sigma_{a_n}} \tag{44}$$

To solve the matrix equations for the power series, (30) and (34), two computer programs have been written in APL language and are shown in Appendix 3.

The programs are conversational in nature and are suitable to be executed with a remote time sharing terminal. In addition to solving the equations, the programs will recalculate the data, show the difference between the observed and calculated points, and show a plot of the observed and calculated (x,y) points.

The programming was simplified by using sub-programs available in the system for matrix inversion, data tabulation, and plotting.

The program for determining the coefficients of a power series without a constant is labeled FITTING and coded HARRYFIT. The program for determining the coefficients of a power series with a constant is labeled THERMOFIT and is also coded HARRYFIT. This latter program also integrates the power series and evaluates the integral from x = 0 to x = 1. The need for THERMOFIT will be shown later.

In both of these programs the order of the equation must be specified and is limited only by the core capacity of the computer. In selecting the order of the equation to best

represent the data, the following principles were found to give the best results:

- use minimum number of terms where all coefficients have greater than 95.0% confidence. (t approximately equal to 2.00, with the degrees of freedom involved here)
- t values appear in descending order.
- values for first order coefficient (slope at x = 0) and intercept are reasonable when compared to plot.

An example of the output from these programs is also in Appendix 2. APL programs for calculating partial pressure of solute (p_2), activity coefficient of solvent (γ_1), activity coefficient of solute (γ_2), and $\log(\gamma_2/\gamma_1)$, entitled CONVERT and THERMO, are included in Appendix 2.

Thermodynamic Consistency

In order to establish confidence that the data used in this thesis were accurately obtained by the original investigators, the Redlich-Kister test for thermodynamic consistency[12,17,34,35] was applied to all systems. The test is based on the Gibbs-Duhem expression for excess free energy and defines as the necessary condition for thermodynamic consistency for isothermal systems:

$$\int_0^1 \log(\gamma_2/\gamma_1)\, dx_{21} = 0 \qquad (45)$$

where the activity coefficient, γ, is given by

$$\gamma = \frac{x_v p_{12}}{x_1 p_o} \qquad (46)$$

x_v = mole fraction vapor

x_l = mole fraction liquid

p_{12} = total pressure

p_o = pressure at $x_{21} = 1$

(Where p_o was not given in the data, it was estimated graphically from a plot of p_{12} vs. x_{21})

Figure 2 shows the typical form of a plot when equation (45) is applied to good data.

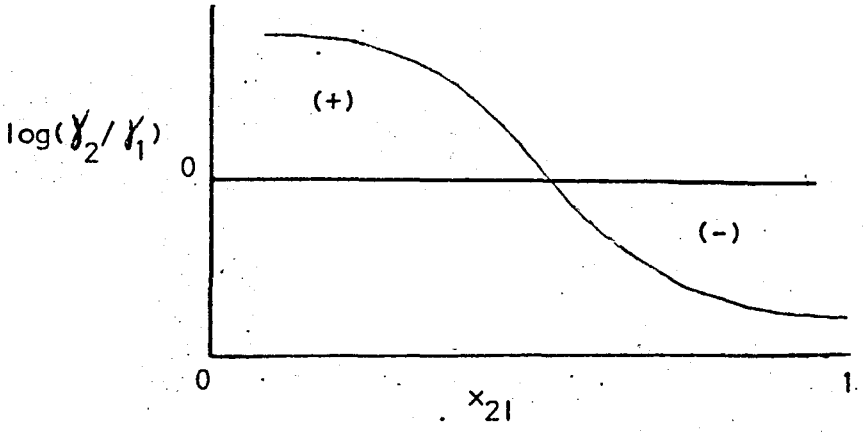


FIGURE 2

Equation (45) is satisfied when the ratio of the positive and negative areas under the curve is 1, thus making the value of the total integral zero. Jaques[17] has graphically integrated the reference system, isopropyl alcohol/benzene at 45°C and reports a ratio of 1.01 as being a satisfactory value for thermodynamic consistency.

The problem now presented is one of establishing the relationship

$$\log(\gamma_2/\gamma_1) = f(x_{21}) \tag{47}$$

and integrating this relationship over the interval zero to one.

$$\int_0^1 \log(\gamma_2/\gamma_1)\,dx_{21} = \int_0^1 f(x_{21})\,dx_{21} \qquad (48)$$

Using the curve fitting principles outlined in the previous section, a power series in x_{21} can again be used to determine $f(x_{21})$ in (47). Applying (30) to (47) gives

$$\log(\gamma_2/\gamma_1) = a_o + a_1 x_{21} + a_2 x_{21}^2 \ldots. \qquad (49)$$

Since no boundary conditions are known (49) can not be modified. Equation (49) can now be integrated and the integral evaluated from x = 0 to x = 1.

$$\int_0^1 \log(\gamma_2/\gamma_1)\,dx = \int_0^1 (a_o + a_1 x_{21} + a_2 x_{21}^2 \ldots)dx$$

$$= a_o x + \frac{a_1 x_{21}^2}{2} + \frac{a_2 x_{21}^3}{3} \cdots \Bigg|_{x=0}^{1}$$

$$= a_o + \frac{a_1}{2} + \frac{a_2}{3} \cdots \qquad (50)$$

The standard error of this estimate is given by equation(43). Applying this to equation (50), we have

$$\int_0^1 \log(\gamma_2/\gamma_1)\,dx = \int_0^1 (f(x) \pm \sigma_{est})\,dx$$

$$= \int_0^1 f(x)\,dx \pm \int_0^1 \sigma_{est}\,dx$$

$$= \int_0^1 (f(x))dx \pm \sigma_{est} \int_0^1 dx$$

$$= \int_0^1 (f(x))dx \pm \sigma_{est} \qquad (51)$$

where $f(x) = a_o + a_1 x_{21} + a_2 x_{21}^2 \ldots$

The standard error of the estimate, (equation (49), is there-

for the standard error of the integral, (equation 50), over the range discussed.

Fitting the data of Jaques[17] to an eighth order polynomial gives

$$A_J = \int_0^1 \log(\alpha_2 / \alpha_1) = 0.0066$$

with a standard error of ±0.0005. With this reference as a guide, systems where the value of the integral was significantly greater than ±0.01 were considered not to be thermodynamically consistent. Data which did not meet this test were ignored in this work.

IV. HENRY'S LAW CONSTANT

The data studied in this work are all binary systems with a non-polar solvent. The principle solvent used was benzene, but in order to involve a greater number of compounds, systems with cyclohexane and carbon tetrachloride solvents were used. All data were taken from the literature and are cited in Appendix 1.

From these isothermal vapor-liquid equilibrium studies, three pieces of data are needed and are generally available over the whole concentration range:

- total pressure (p_{12})
- mole fraction solute in the liquid (x_{2l})
- mole fraction solute in the vapor (x_{2v})

Other necessary data can now be calculated:

- activity coefficient for solute (γ_2) and solvent (γ_1) which are needed in equation (46) for testing thermodynamic consistency
- partial pressure of solute (p_2)

$$p_2 = x_{2v} p_{12} \tag{52}$$

Henry's Law states that in dilute solutions, the vapor pressure of a component is proportional to its mole fraction[18].

$$p_2 = k_H x_2 \tag{53}$$

If the behavior demonstrated by the dilute state continued through finite concentrations to the pure state ($x_2 = 1$), it would follow Henry's Law and the vapor pressure of the pure component would be Henry's Law constant, k_H. This was shown in Section III.

The p_2 vs. x_{21} curve can be described by a power series in x_{21}. In this case equation (34) would be used:

$$p_2 = a_1 x_{21} + a_2 x_{21}^2 + a_3 x_{21}^3 \ldots$$

The initial constant term is omitted since we have a boundary condition where p_2 must be zero when x_{21} is zero. After the constants are determined according to the procedures in Section III, the equation may be differentiated and evaluated at $x_{21} = 0$ to give:

$$\frac{d\ f(x)}{dx} = a_1 + 2a_2 x + 3a_3 x^2 \ldots \tag{54}$$

$$\lim_{x_{21}\ 0} \frac{d\ f(x)}{dx} = a_1 = k = p_o \tag{55}$$

From equation (29), this a_1 is the k_H of Henry's law and reflects molecular behavior in the infinitely dilute state projected to the pure state.

Methods for determining the standard error in this coefficient have already been discussed in Section III.

The values of the Henry's law constants $k_H = p_2^o$ are listed in Table 4 in the following section.

V. IDEALIZED HEAT OF VAPORIZATION

From the schematic for the vaporization of ethanol presented in section II we see that

$$\Delta H^{o} = \Delta H_{v} - \Delta H_{s}^{\infty} + \Delta H_{T}$$

The enthalpy of diluting a gas from the pure state to the infinitely dilute state is given by

$$\mu_{J.T.} = \frac{-1}{c_p}\left(\frac{\partial H}{\partial P}\right)_{T}$$

where c_p is the Joule Thomson coefficient[18].

Assuming c_p and $\mu_{J.T.}$ to be constant and integrating, we have

$\Delta H_T = -c_p \mu_{J.T.} \Delta P \cong 0$ for small P. We therefore have

$$\Delta H^{o} = \Delta H_{v} - \Delta H_{s}^{\infty}$$

To understand ΔH^{o} more fully, consider what happens when a solute molecule is vaporized from a solution.

In order for a molecule to move from the liquid to the vapor state it must attain an adequate increment of kinetic energy and it must overcome the attraction of surrounding liquid molecules. The energy required for this is the heat of vaporization. The kinetic energy term is mass dependent and thus should correlate with molecular weight. By keeping the surrounding molecular environment the same the second effect should be constant. An ideal heat of vaporization under these conditions would be expected to correlate well with molecular weights, a correlation not found with heats of vaporization

of the pure substances. The infinitely dilute state in a non-polar solvent is one in which the molecular environment of a solute molecule is constant, hence solute heats of vaporization under these conditions are expected to correlate well with molecular weight.

In section IV we found k_H and interpreted it as vapor pressure, p_2^o, the solute would have if it had the same molecular environment when pure as in the infinitely dilute solution. Heats of vaporization calculated from these values of p_2^o by means of the Clausius-Clapeyron equation

$$\log p_2^o = \frac{\Delta H_2^o}{2.303\ R}\ .\frac{1}{T} + C \qquad (56)$$

would fulfill the requirements for an ideal heat of vaporization that would be expected to show a correlation with molecular weight.

Figures 3 - 18 show plots of $\log p_2^o$ versus 1/T for the systems listed in Table 4. The values of ΔH_2^o determined from these plots are given in Table 5 and compared there with the standard heat of vaporization.

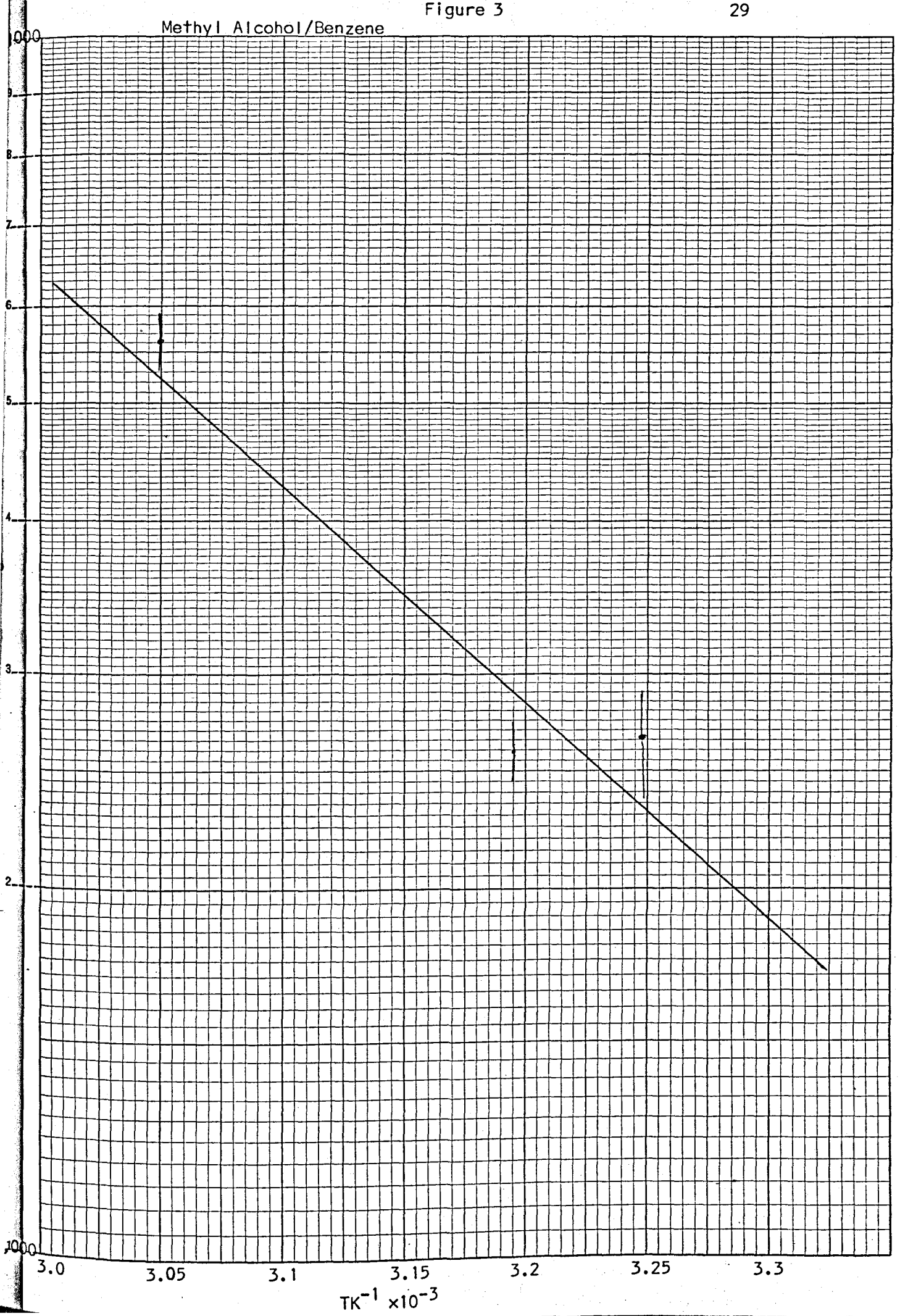
TABLE 4

SYSTEM component 2/component 1	M.W.	T°C	P_2^o	THERMODYNAMIC CONSISTENCY A_y
Methyl Alcohol/Benzene	32	35	2654.9	0.1085
		40	2591.0	0.1961
		55	5636.4	0.0759
Ethyl Alcohol/Benzene	46	40	1468.7	-0.0116
		50	2347.2	-0.0116
Ethyl Alcohol/Cyclohexane	46	10	496.6	-0.0073
		20	823.8	0.0105
		25	860.1	-0.0663
		30	1409.9	0.0253
Butyl Alcohol/Benzene	74	25	29.8	-0.5561
		45	215.0	-0.3220
Isopropyl Alcohol/Benzene	66	25	296.6	0.0376
		45	1075.9	0.0395
Fluorobenzene/Cyclohexane	96	50	382.0	-0.0010
		60	529.6	0.0127
		70	740.2	0.0059
Cyclohexane/Benzene	84	40	294.7	0.0065
		70	857.9	0.0113
Chloroform/Carbon Tetrachloride	119	40	416.1	-0.0049
		55	692.9	-0.0049
Carbon Tetrachloride/Benzene	153	40	237.9	0.0008
		40	246.1	-0.3405
		70	680.5	-0.0014
Ethyl Ether/Benzene	74	20	1126.7	0.0484
		35	1949.2	0.0316
Methane/Benzene	16	40	6627.5	-0.4780
		60	7392.5	-0.3629
		80	7056.3	-1.4621
		100	9200.5	-0.6211
		120	10636.1	-0.8730
		150	8407.7	-0.4680
Propane/Benzene	44	38	31512.6	0.7158
		71	49741.1	-0.2230
		104	56932.5	-0.4445
		138	71315.0	0.6216
		171	90916.6	-88.6252
		204	90831.8	-4.1790
Heptane/Benzene	100	60	371.2	0.0199
		80	702.3	0.0316

TABLE 4 (continued)

SYSTEM component 2/component 1	M.W.	T°C	P_2^o	THERMODYNAMIC CONSISTENCY A_y
Octane/Benzene	114	55	111.3	0.0007
		65	150.6	0.0019
		75	194.7	0.0128
Toluene/Benzene	92	120	973.4	-29.7654
		160	4399.6	0.1109
		200	7488.1	0.0300
		240	12943.6	0.0469
		280	32717.4	0.1334
Tetraethylsilane/Benzene	144	20	10.42	0.0197
		35	19.19	0.0058
		50	35.89	0.0061
Ethylene Dichloride/Benzene	99	20	374.3	0.1348
		45	244.2	0.0054
		70	542.6	0.0024

Figure 3


Methyl Alcohol/Benzene
1000
9
8
7
6
5
4
3
2
1000
3.0
3.05
3.1
3.15
3.2
3.25
3.3
TK^{-1} x10^{-3}

Ethyl Alcohol/Cyclohexane (A)
Ethyl Alcohol/Benzene (B)

Figure 4

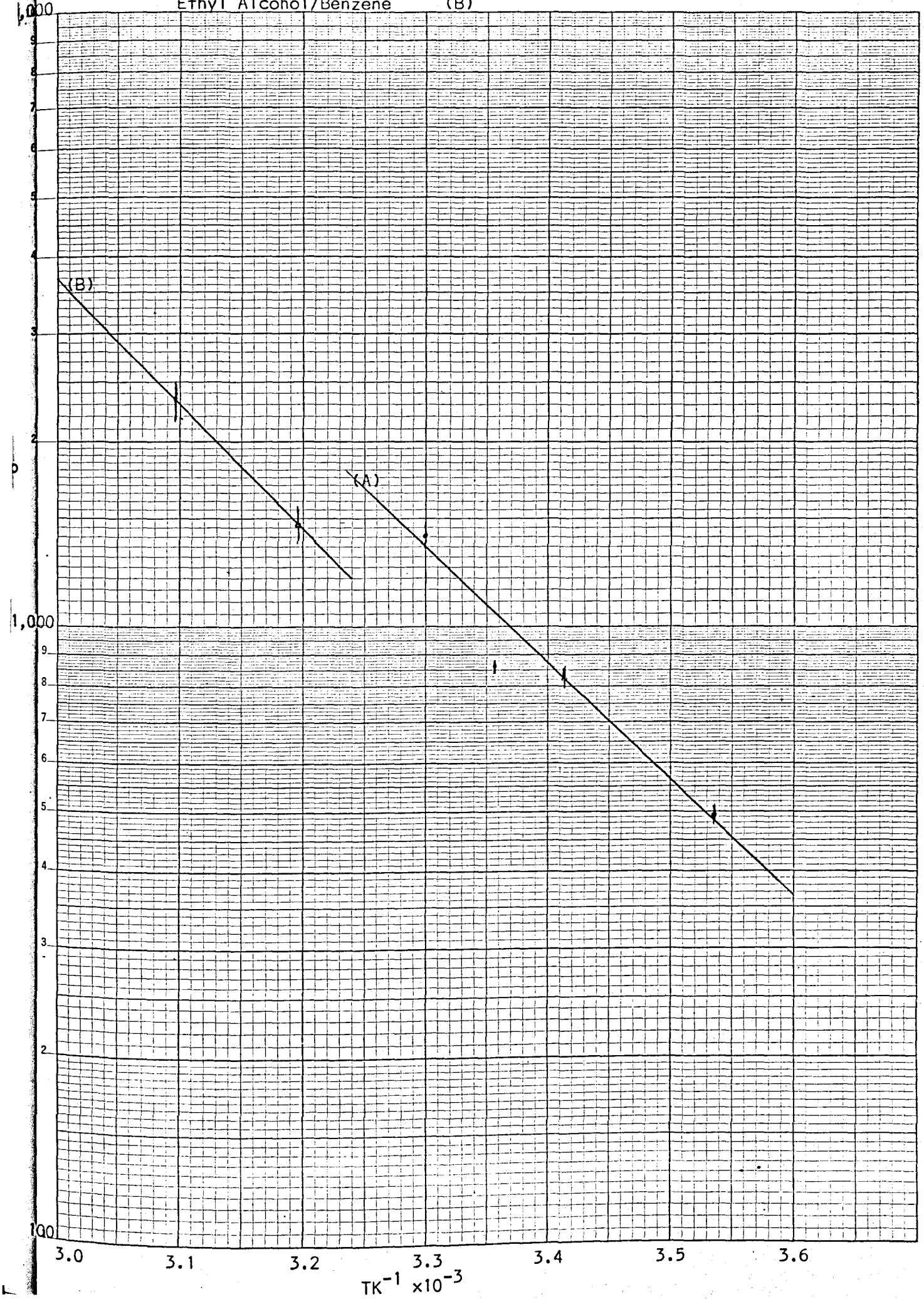


Figure 5

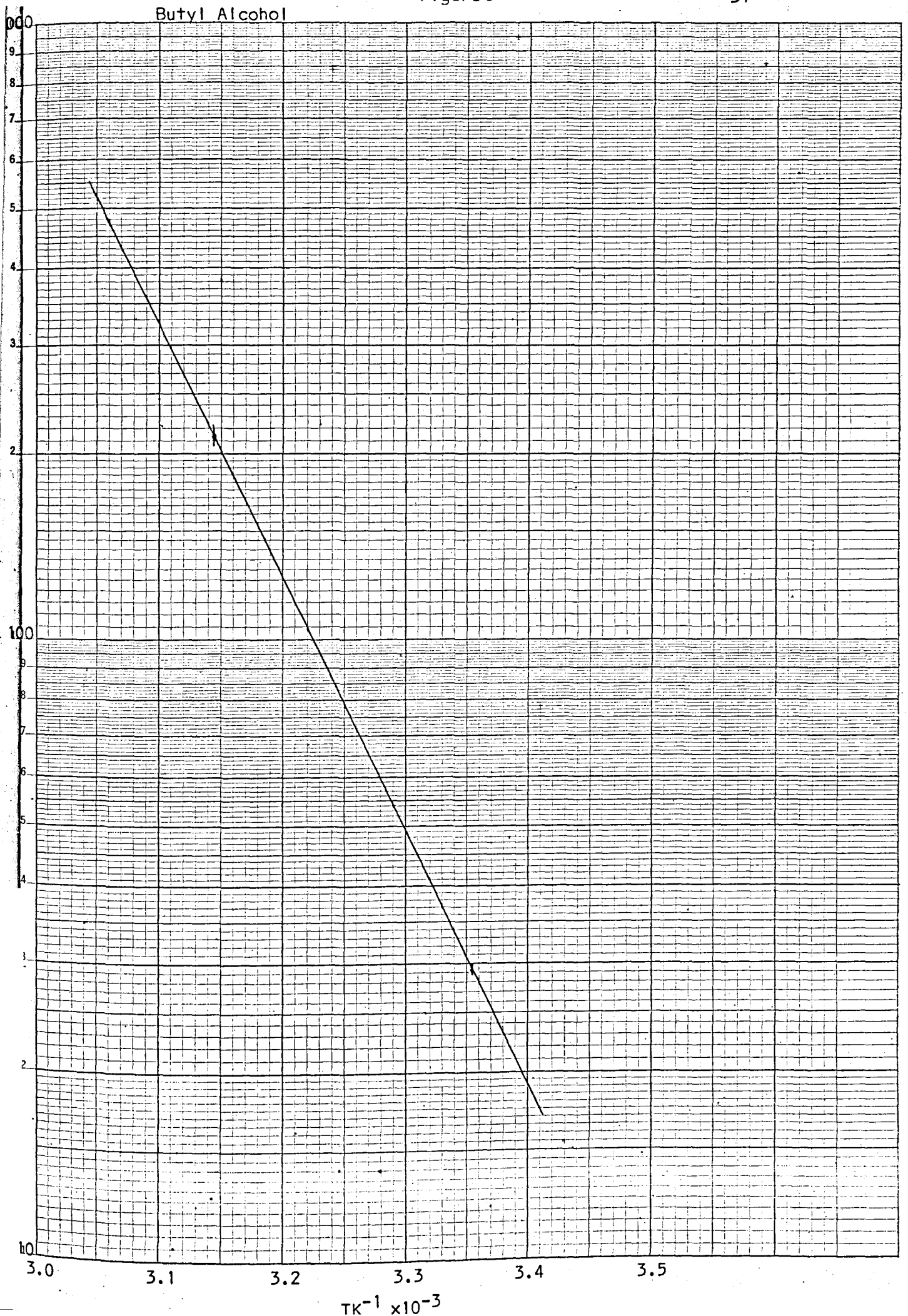

Butyl Alcohol
1000
900
800
700
600
500
400
300
200
100
90
80
70
60
50
40
30
20
10
3.0
3.1
3.2
3.3
3.4
3.5
TK^{-1} x10^{-3}

Figure 6

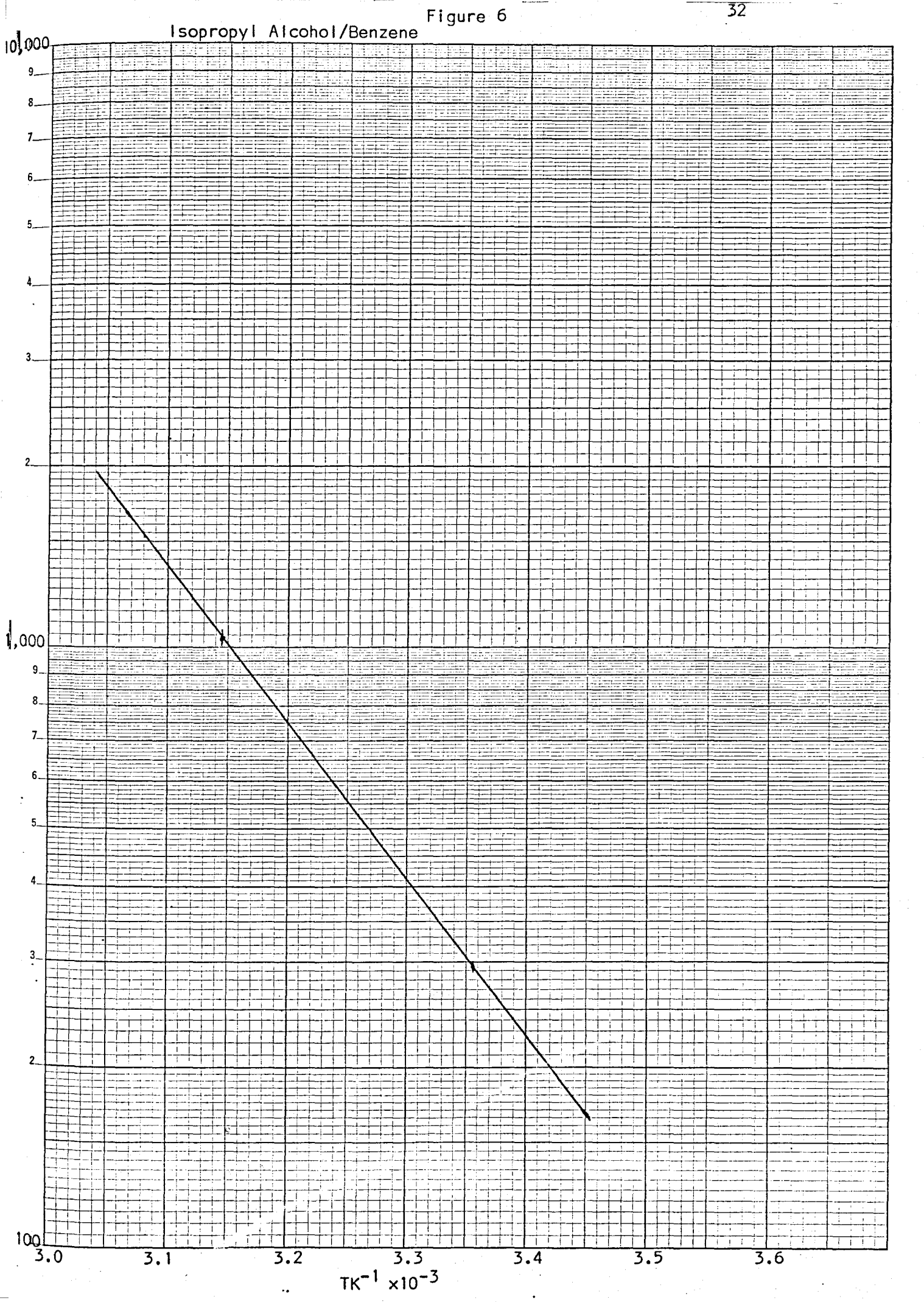

Isopropyl Alcohol/Benzene
10,000
9
8
7
6
5
4
3
2
1,000
9
8
7
6
5
4
3
2
100
3.0
3.1
3.2
3.3
3.4
3.5
3.6
TK^{-1} x10^{-3}

Figure 7

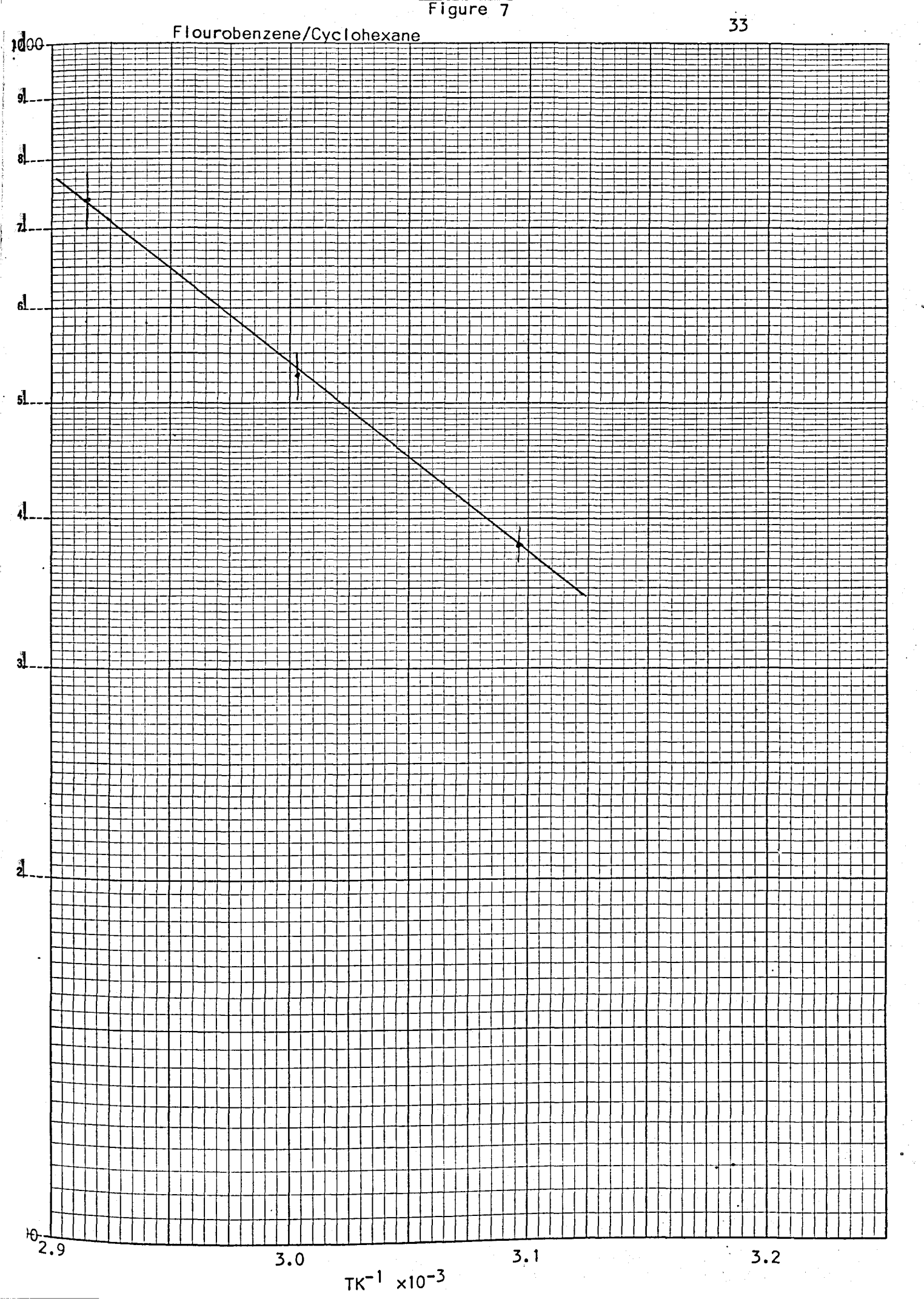

Flourobenzene/Cyclohexane
1000
9
8
7
6
5
4
3
2
10
2.9
3.0
3.1
3.2
TK^{-1} x10^{-3}

Figure 8

Cyclohexane/Benzene

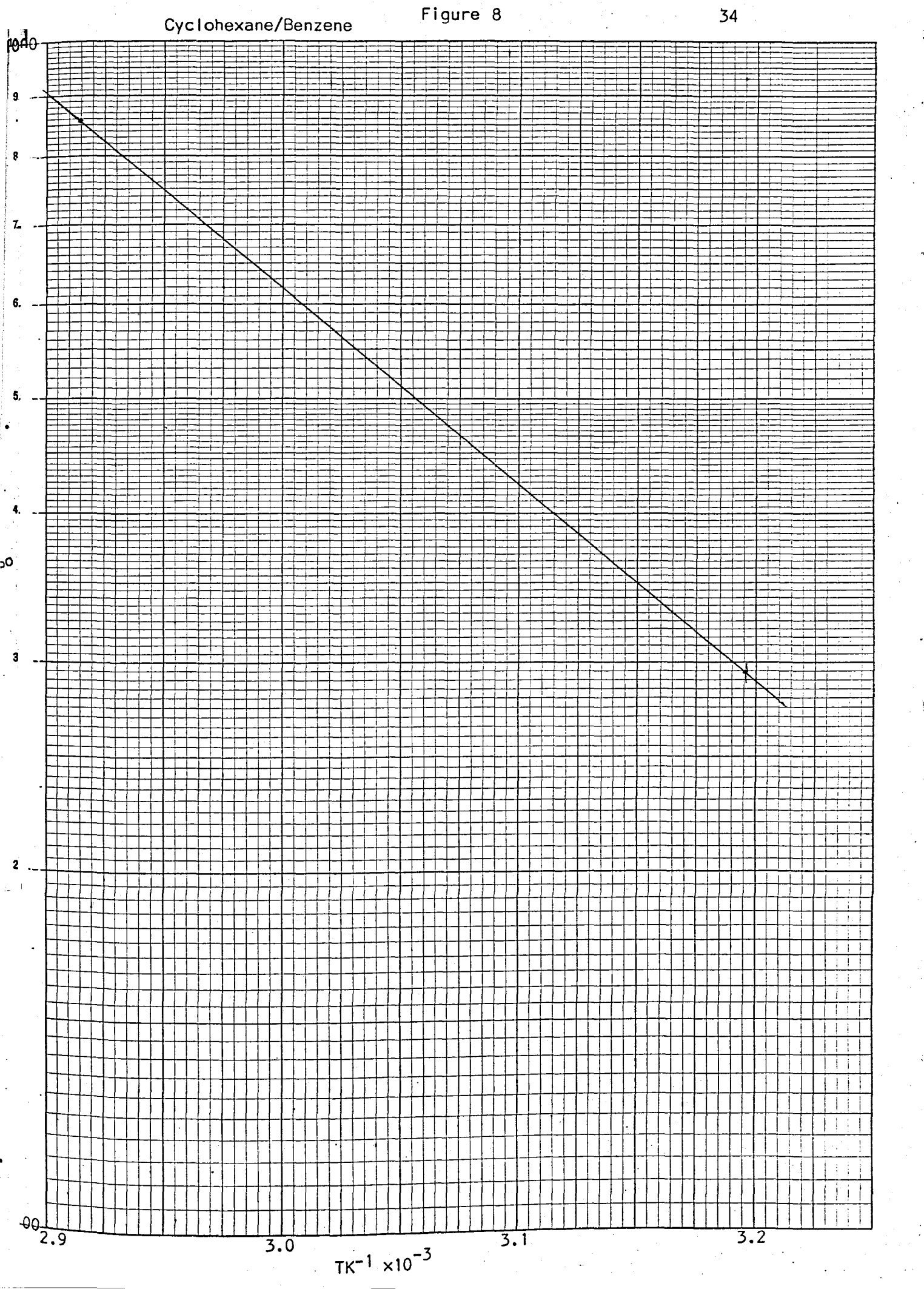


Figure 9

Chloroform/Carbon Tetrachloride

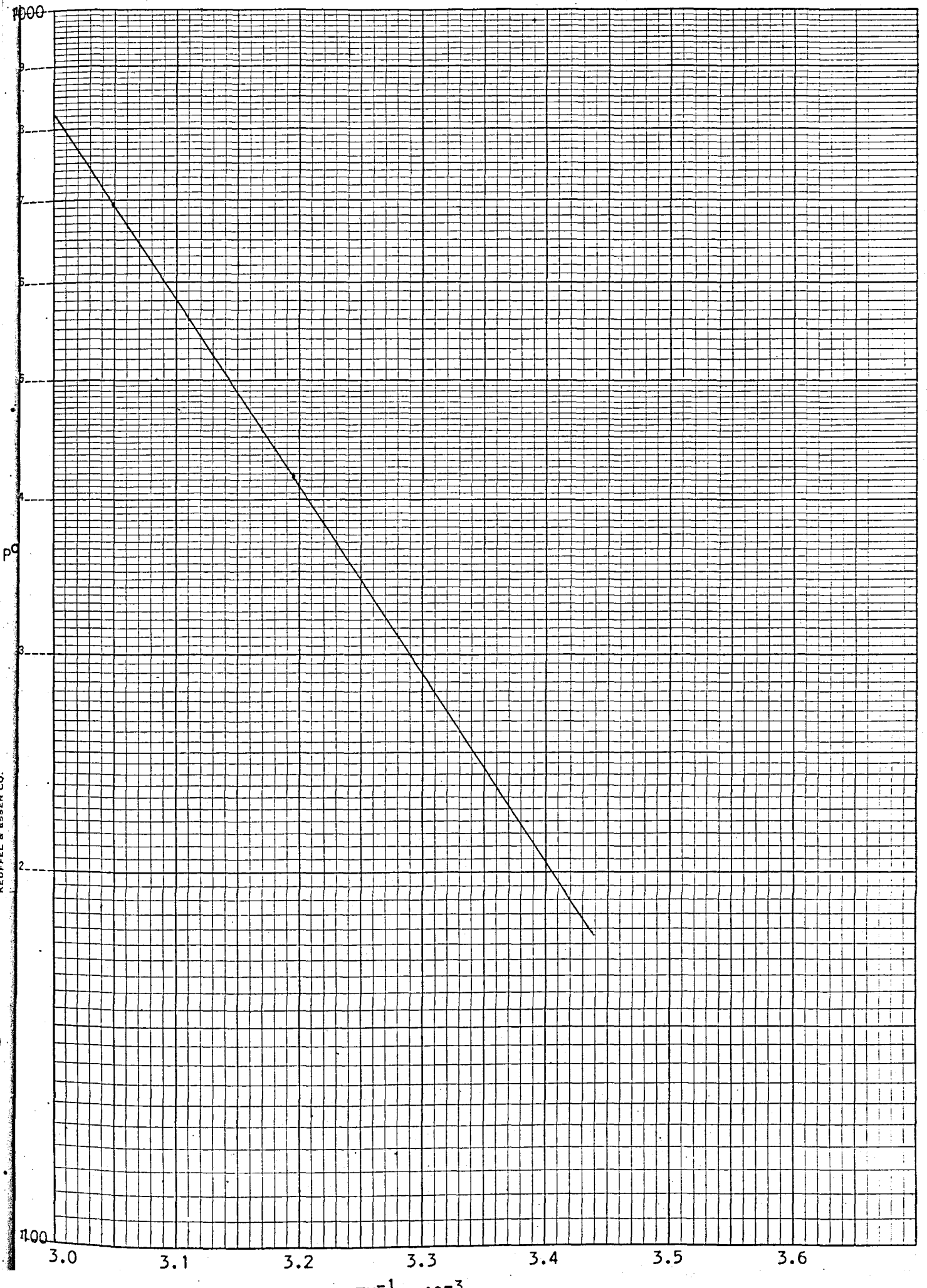


Figure 10

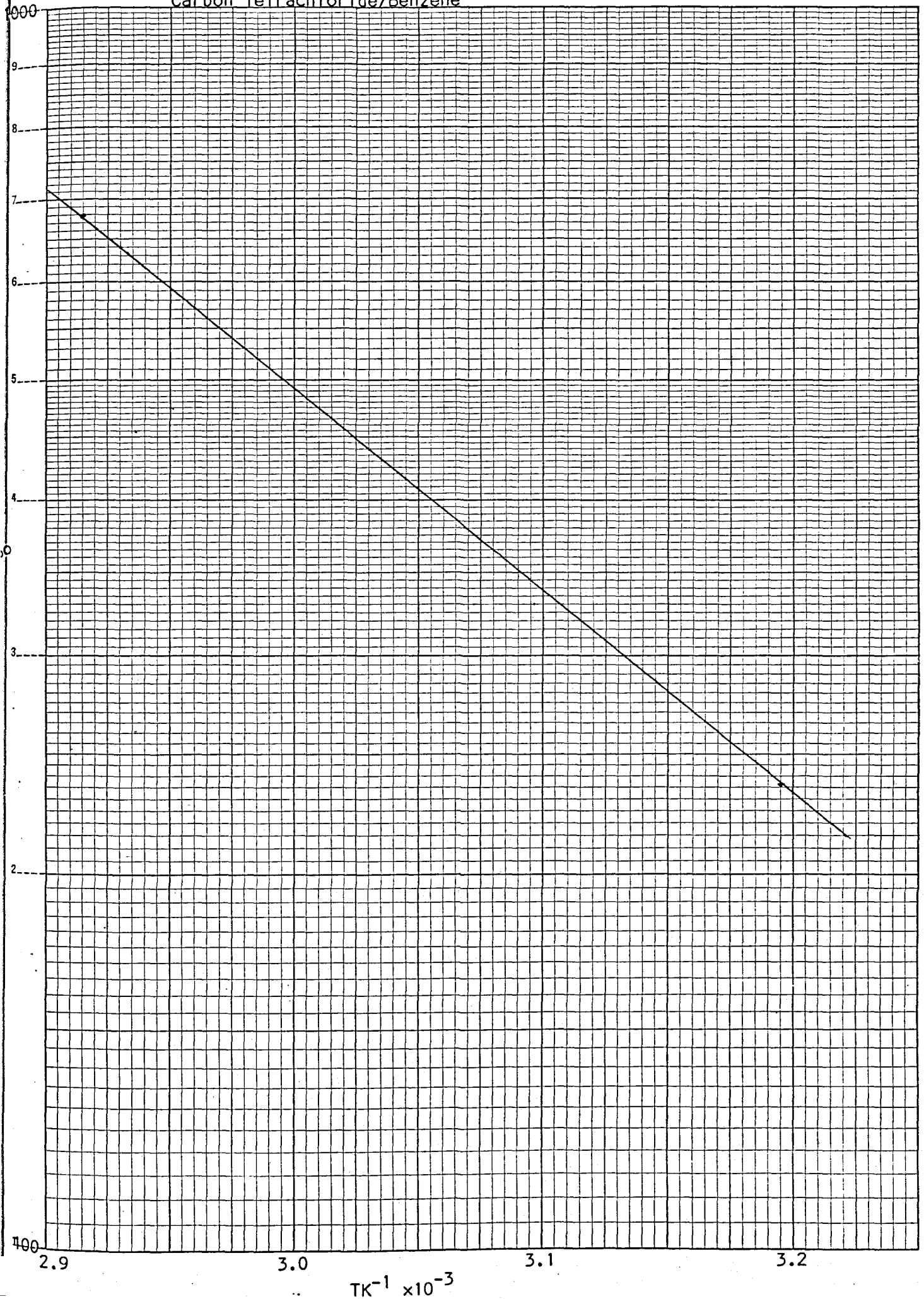

Carbon Tetrachloride/Benzene
1000
9
8
7
6
5
4
3
2
1100
2.9
3.0
3.1
3.2
$TK^{-1} \times 10^{-3}$

Figure 11

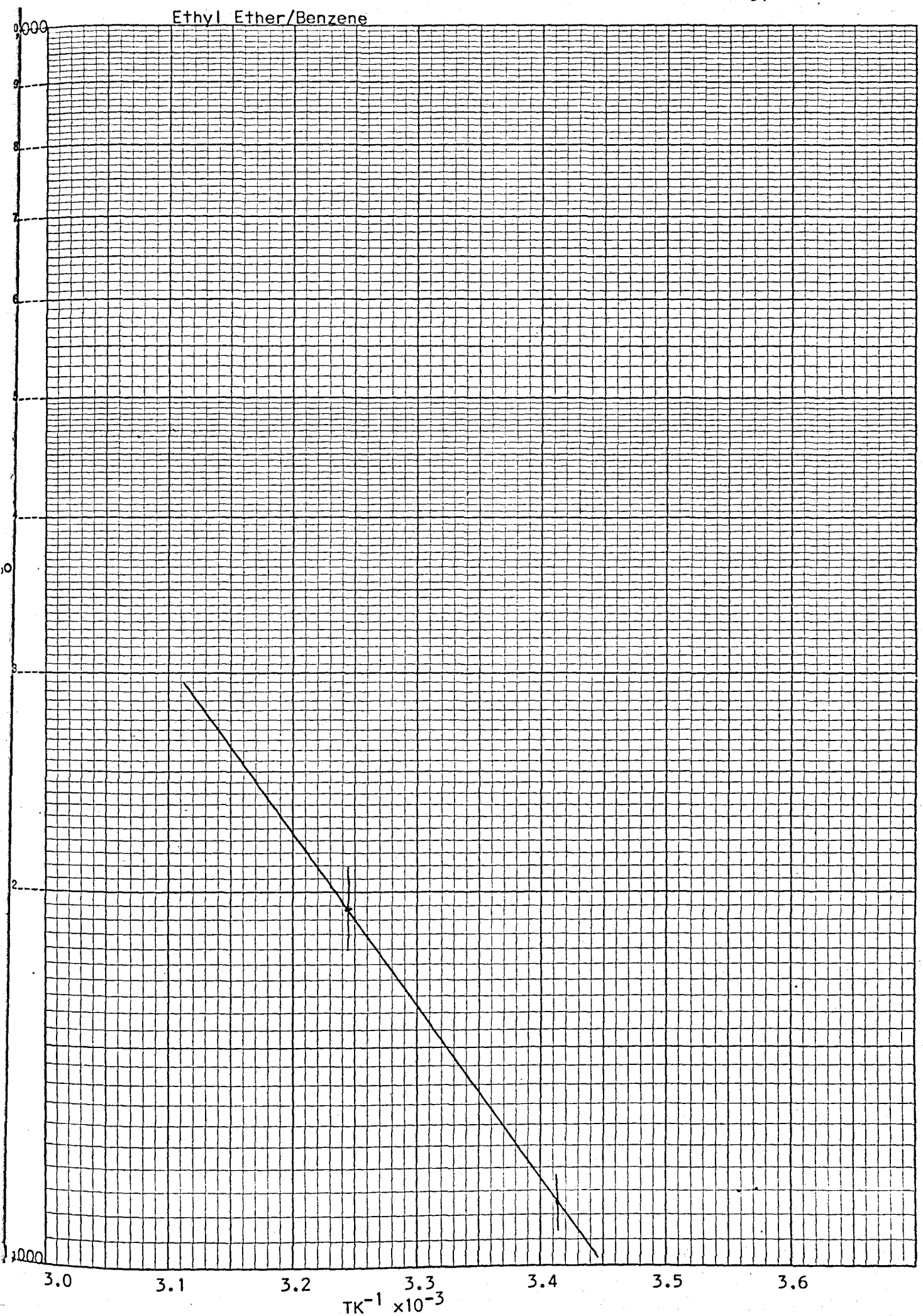


Figure 12

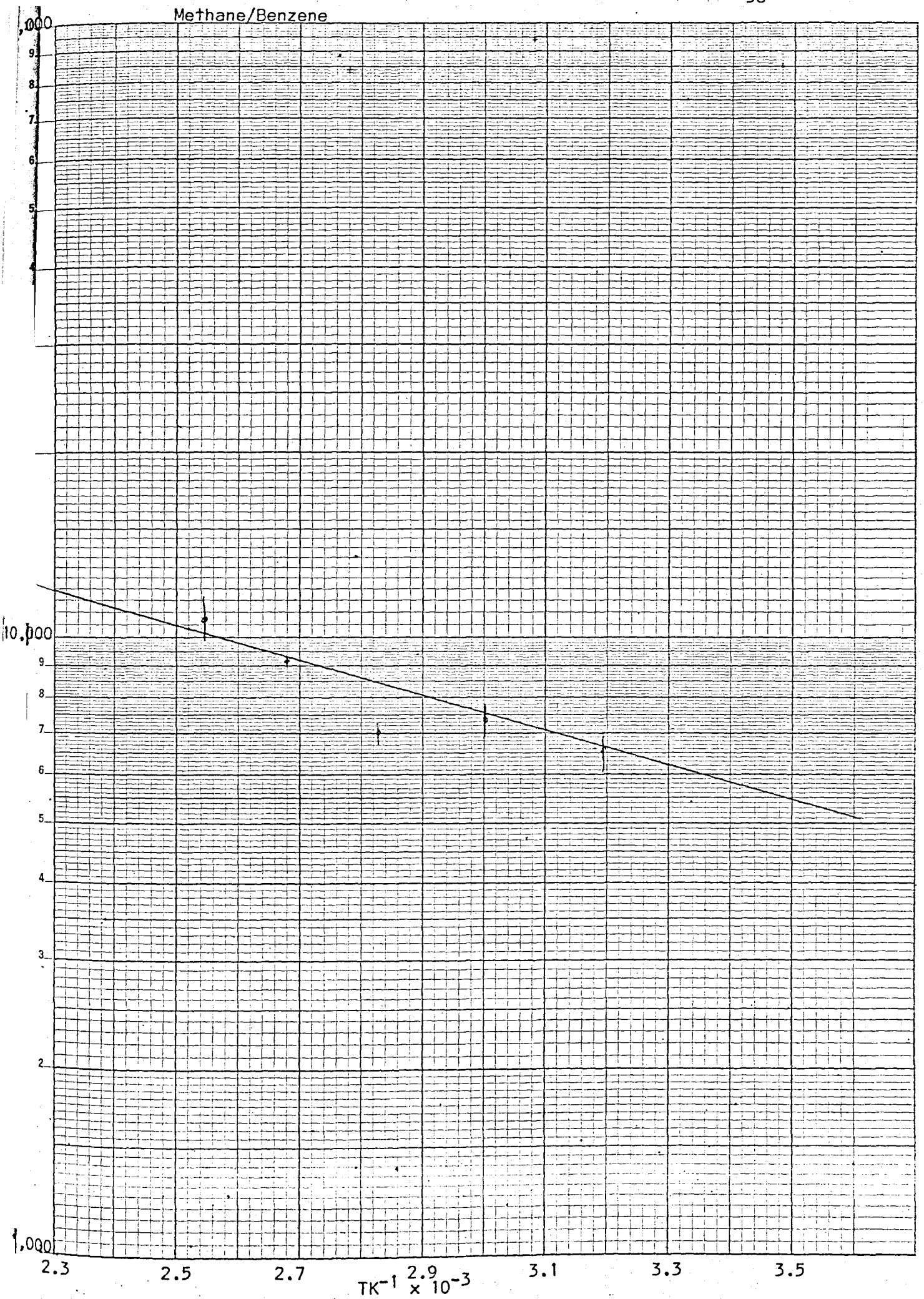
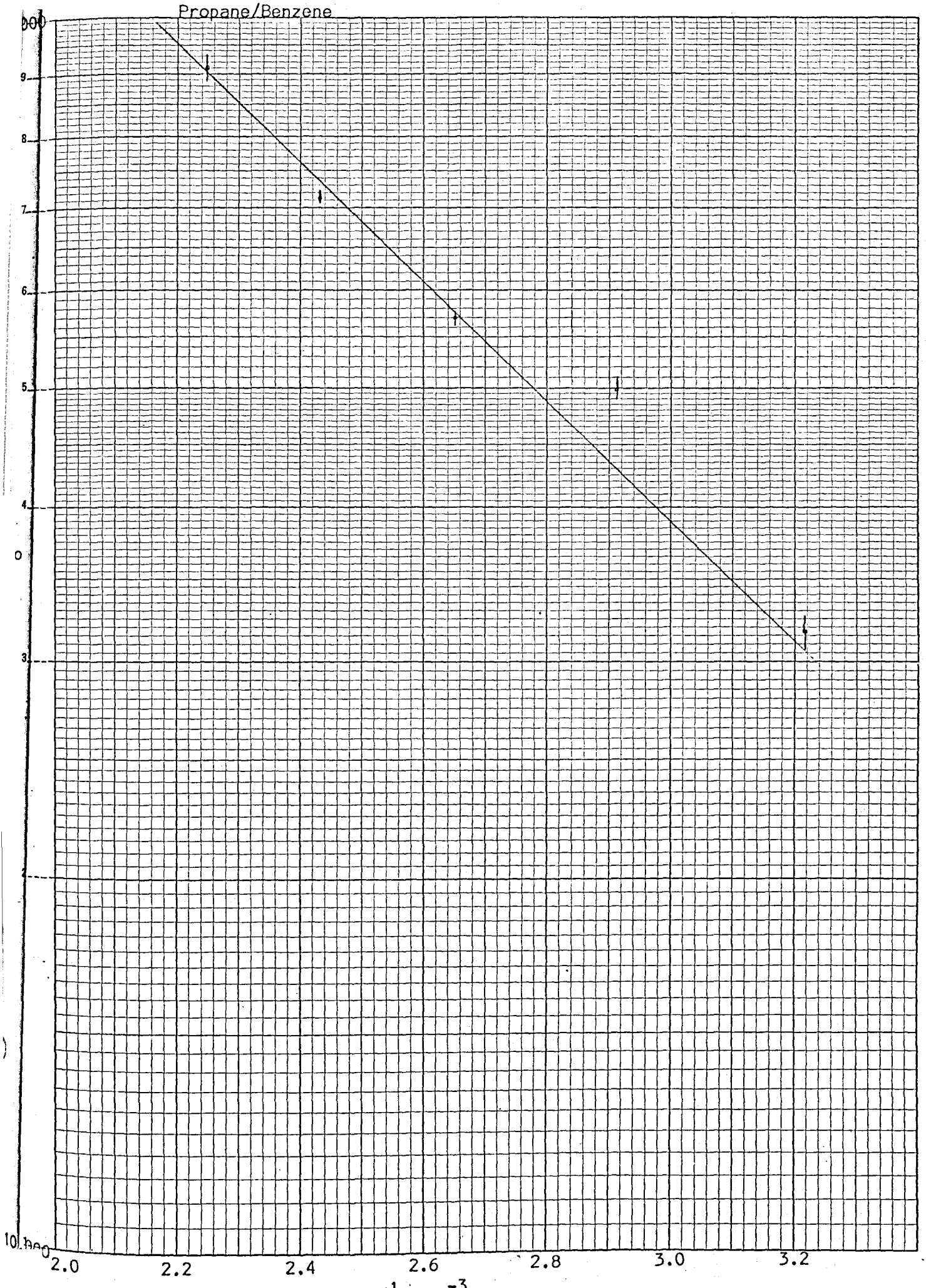

Methane/Benzene
10,000
9
8
7
6
5
4
3
2
1,000
2.3
2.5
2.7
2.9
3.1
3.3
3.5
TK⁻¹ x 10⁻³

Figure 13



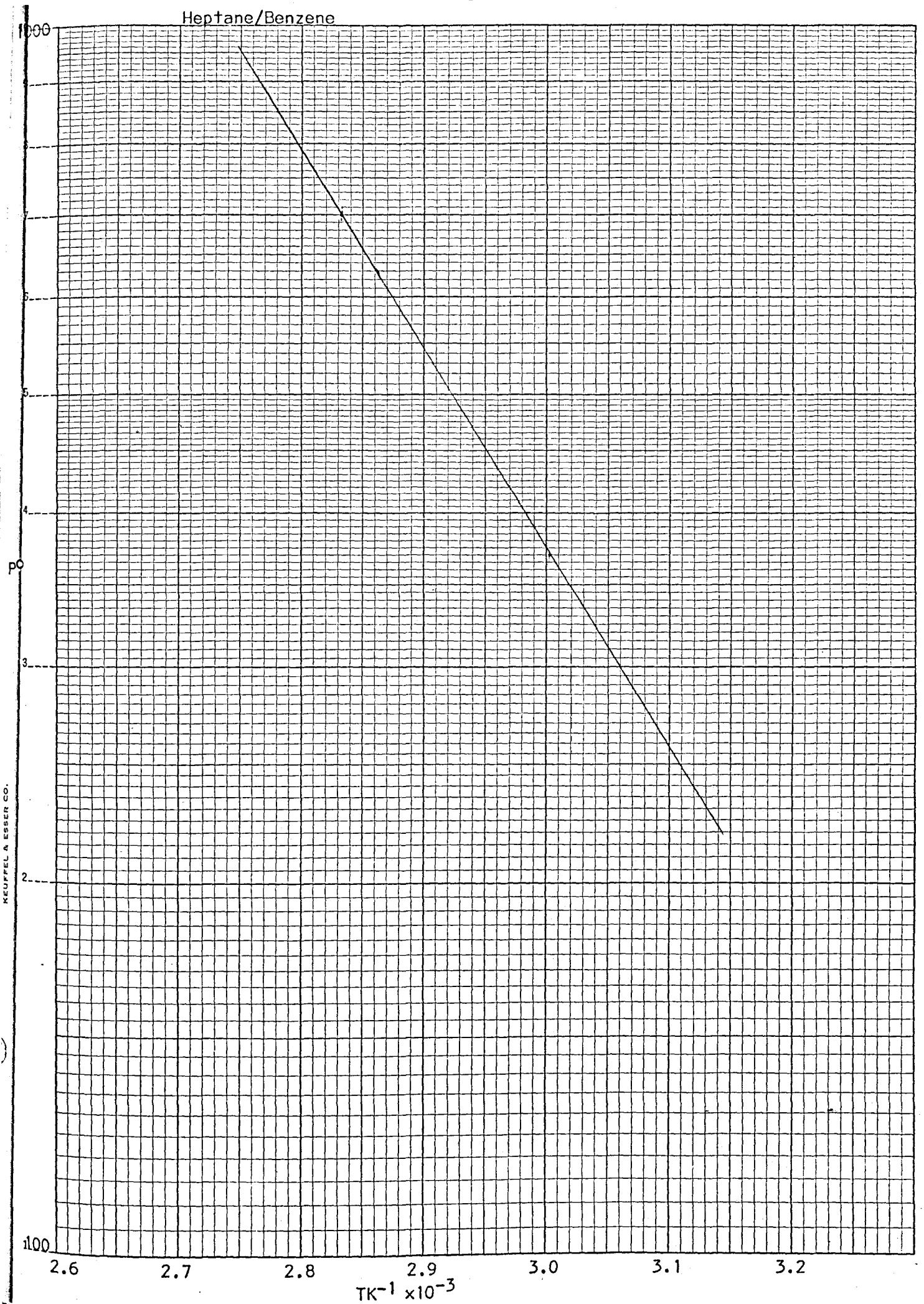
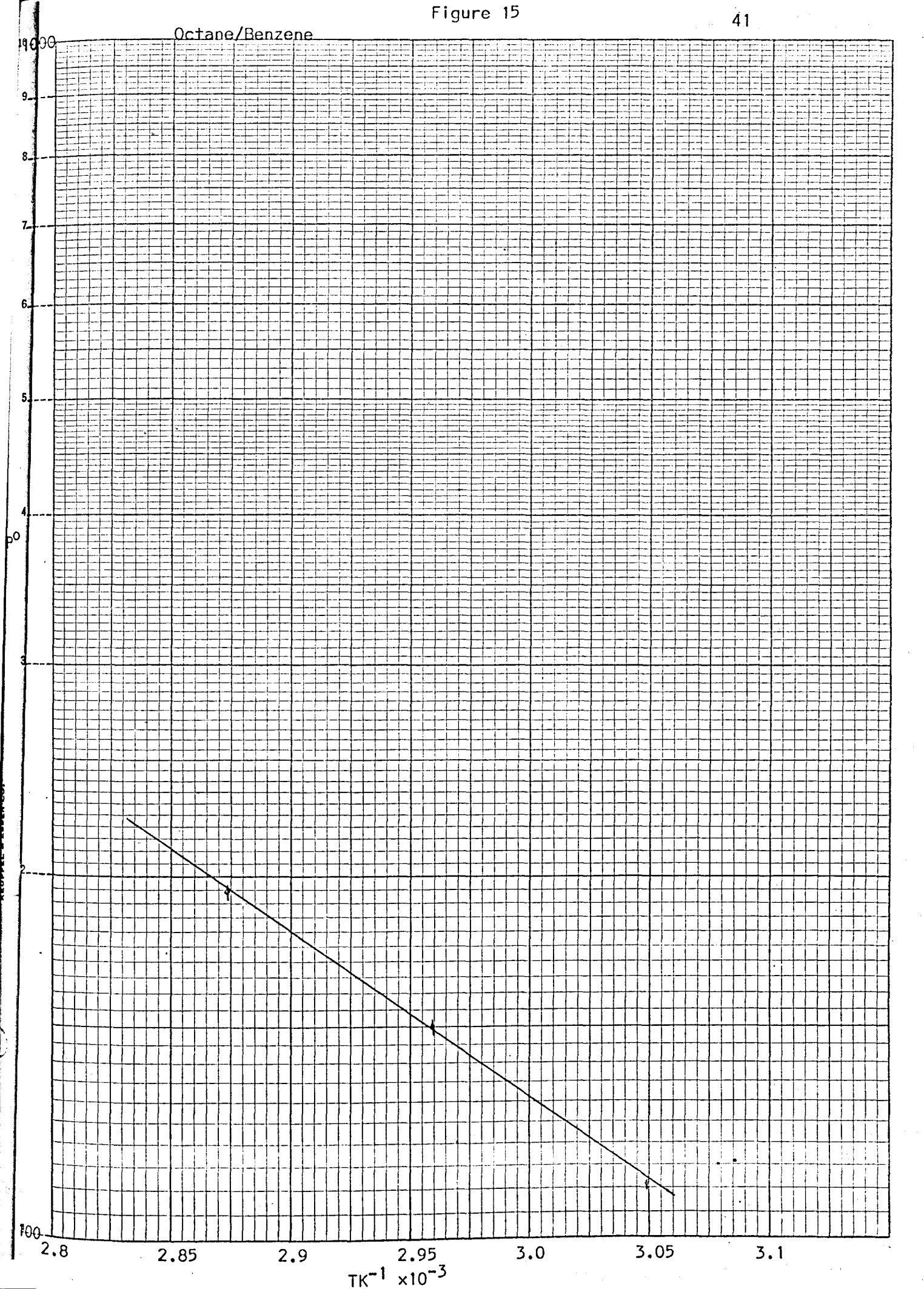
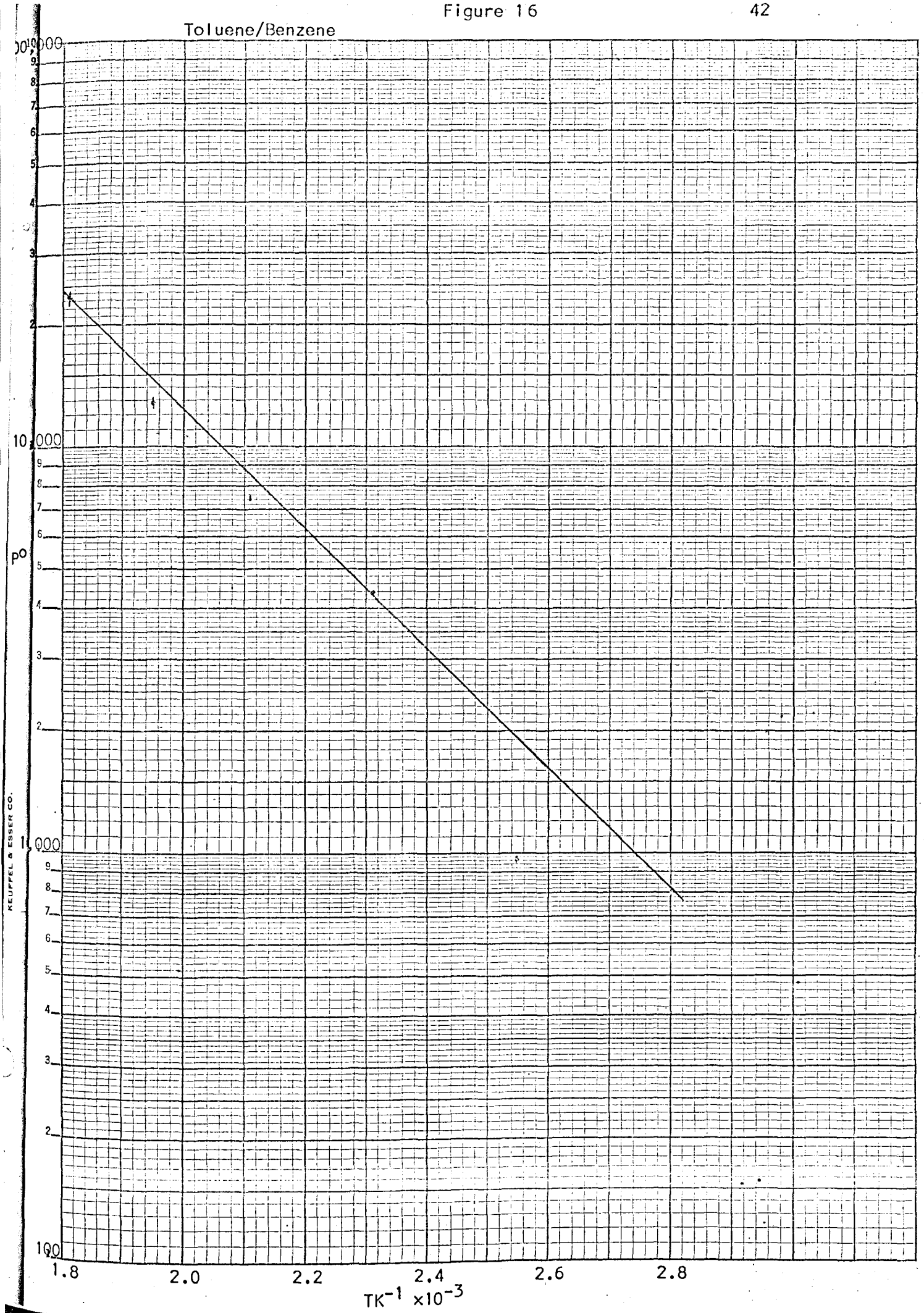

Heptane/Benzene
1000
7
5
5
4
P0
3
2
100
2.6
2.7
2.8
2.9
3.0
3.1
3.2
TK^{-1} x10^{-3}
KEUFFEL & ESSER CO.

Figure 15


Octane/Benzene
10000
9
8
7
6
5
4
P°
3
2
700
2.8
2.85
2.9
2.95
3.0
3.05
3.1
TK^{-1} x10^{-3}


Toluene/Benzene
10,000
9
8
7
6
5
4
3
2
10,000
9
8
7
6
5
4
3
2
1,000
9
8
7
6
5
4
3
2
100
P°
1.8
2.0
2.2
2.4
2.6
2.8
TK⁻¹ x10⁻³
KEUFFEL & ESSER CO.

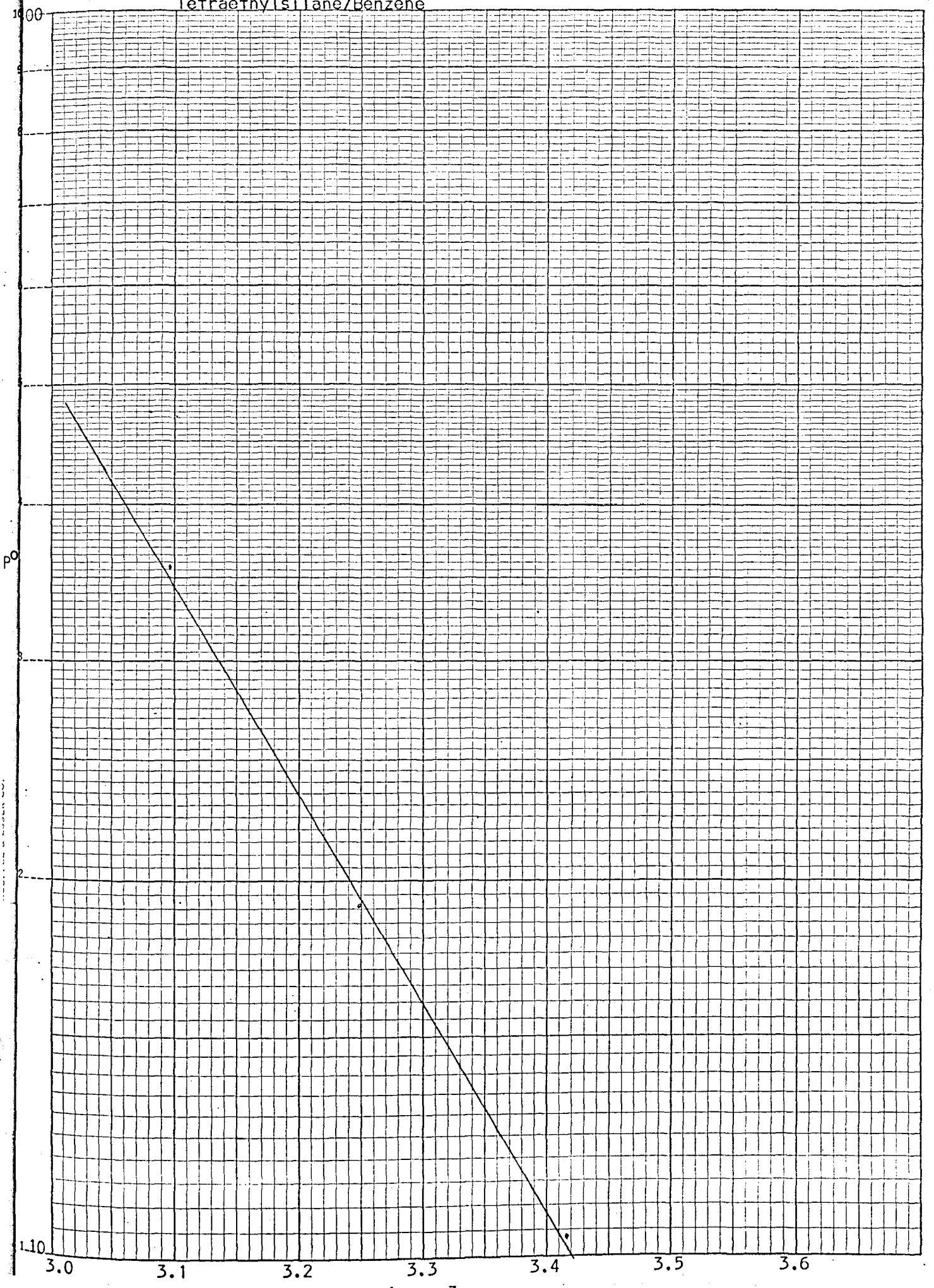

Tetraethylsilane/Benzene
1000
800
600
400
P°
300
200
1.10
3.0
3.1
3.2
3.3
3.4
3.5
3.6
TK⁻¹ ×10⁻³

Figure 18

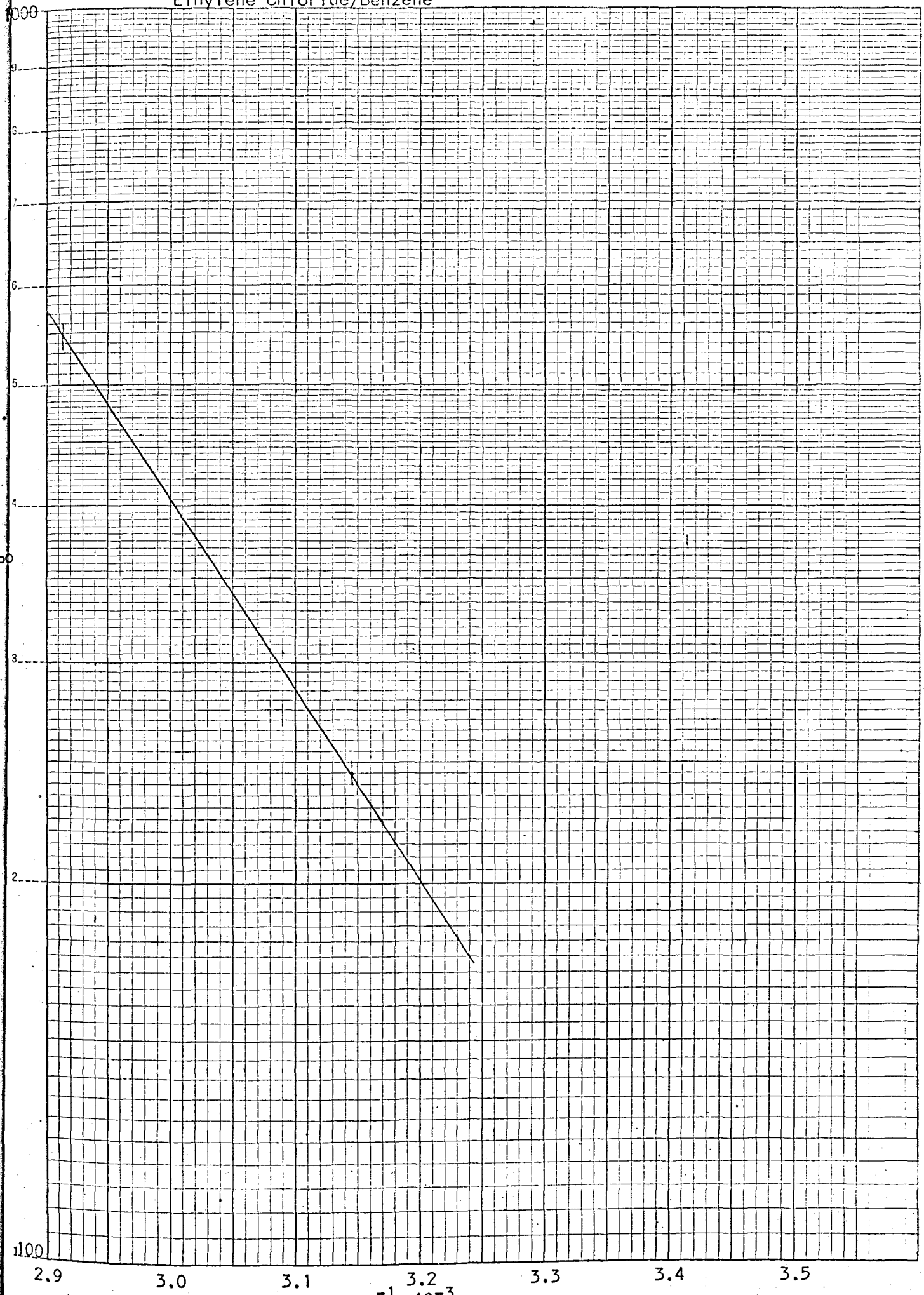

Ethylene Chloride/Benzene
1000
9
8
7
6
5
4
P°
3
2
100
2.9
3.0
3.1
3.2
3.3
3.4
3.5
TK⁻¹ x10⁻³
KEUFFEL & ESSER CO.

TABLE 5

SOLUTE	SOLVENT	M.W.	IDEALIZED ΔH° KCal/mole	STANDARD* ΔH KCal/mole
Methane	Benzene	16	1.25	2.06
Methanol	"	32	7.50	8.94 @ 25°C
Propane	"	44	2.25	4.88
Ethanol	"	46	9.40	10.11 @ 25°C
Isopropanol	"	66	12.14	10.85 @ 25°C
Butanol	"	74	18.61	12.52 @ 25°C
Ethyl Ether	"	74	6.56	6.65
**Cyclohexane	"	84	7.58	7.87
Toluene	"	92	6.63	9.05
**Ethylene dichloride	"	99	6.94	7.9
**Heptane	"	100	7.41	8.72
**Octane	"	114	6.32	9.89
**Tetraethylsilane	"	144	7.74	....
**Carbon tetrachloride	"	154	7.46	7.19
**Ethanol	Cyclohexane	46	8.59	10.11
**Fluorobenzene	"	96	7.23	....
**Chloroform	Carbon tetrachloride	119	6.95	7.94

* Timmermann , J., Physico-Chemical Constants of Pure Organic Compounds, Elsevier Publishing Company(New York), 1950.

Polak, J. and Benson, G.C., Journal of Chemical Thermodynamics, 3, 235(1971)

** System conforms to requirement for thermodynamic consistency outlined in Section III.

VI. CORRELATION TO MOLECULAR WEIGHT

As indicated in Table 5, only nine of the systems conform to the requirements for thermodynamic consistency outlined in Section III. Only these data could therefor be considered for correlation of ΔH^{O} to molecular weight.

Among the data considered to be acceptable for correlation to molecular weight is one system from the family of alcohols. The ΔH^{O} from this binary system, Ethanol/Cyclohexane, seems to separate itself from those of the other eight systems. The separation is more evident when the additional data from the family of alcohols which did not meet the test for thermodynamic consistency are considered. Since there is only one reliable value for ΔH^{O} in the alcohol family, no correlation to molecular weight can be made for this family.

Among the remaining eight values for ΔH^{O}, there are no obvious family separations. These values were therefor correlated to molecular weight as a single group.

Two least squares correlations were made, a linear fit and a log-log fit, with the following results:

$$\Delta H^{O} = 0.0034\, M + 6.81 \tag{57}$$

and

$$\log \Delta H^{O} = 0.0357 \log M + 0.784 \tag{58}$$

Converting equation (58), we have

$$\Delta H^{O} = 6.08\, M^{0.0357} \tag{59}$$

These fits are shown in Figures 19 and 20 respectively.

Figure 19

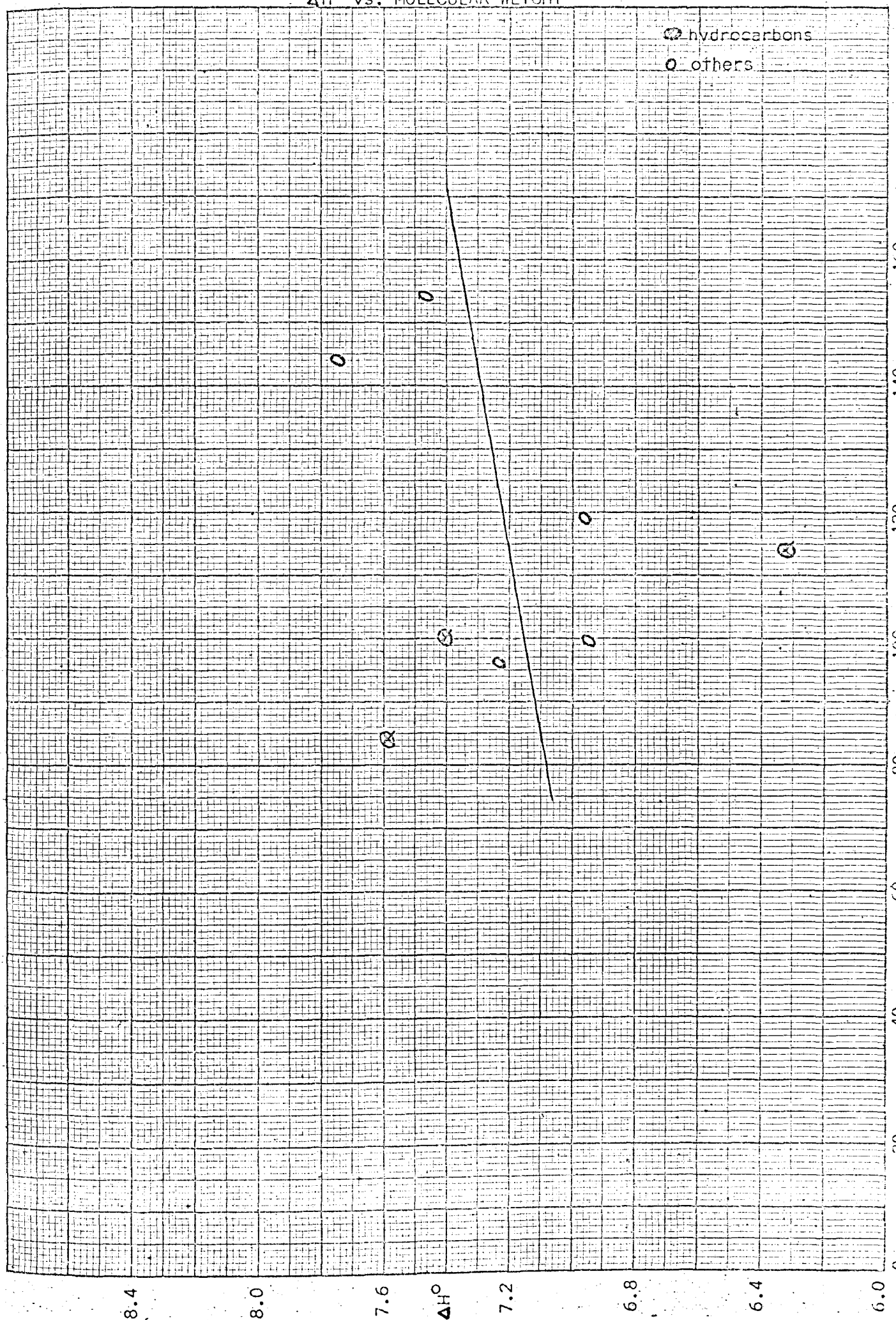
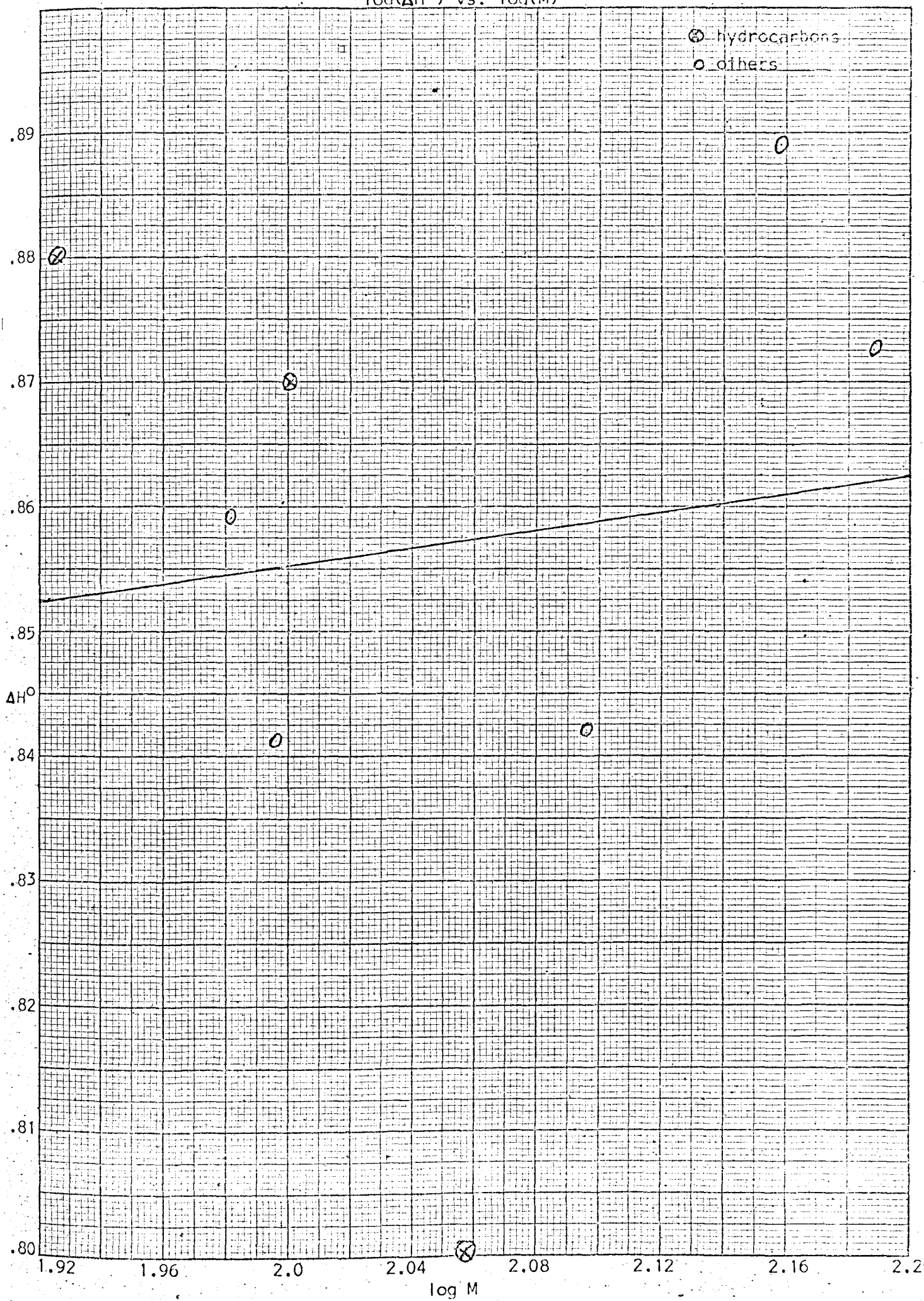

ΔH° vs. MOLECULAR WEIGHT
hydrocarbons
others
ΔH°
8.4
8.0
7.6
7.2
6.8
6.4
6.0
0
20
40
60
80
100
120
140
160
M

Figure 20
$\log(\Delta H^{o})$ vs. $\log(M)$



The log-log fit is the form used by Ibrahim and Kuloor[16] and is represented by equation (21).

$$\Delta H_{vb} = CM^{-n}$$

Since their ΔH_{vb} is expressed in cal/g, it is necessary to multiply by M to convert to cal/mole. The result is

$$\Delta H_{vb} = CM^{(1-n)}$$

Since $n < 1$, the value of the exponent is always positive, thus assuring that ΔH increases as M increases.

For reference, the same least squares fits were made for the corresponding standard ΔH values for the pure substance marked with asterisks in Table 5, with the following results.

$$\Delta H = -0.0116\ M + 9.55 \qquad (60)$$

and

$$\log \Delta H = -0.145\ \log M + 1.209 \qquad (61)$$

Converting equation (61) we have

$$\Delta H = 16.2\ M^{-0.145} \qquad (62)$$

These fits are shown in Figures 21 and 22 respectively.

Since Ibrahim and Kuloor's correlation deals only with homologous series groupings, least squares fits were also made for the standard ΔH for the pure substance of a series of hydrocarbons. The data are listed in Table 6 and the following are the results of the fitting:

$$\Delta H = 0.0653\ M + 1.31 \qquad (63)$$

and

Figure 21

ΔH_{obs} vs. MOLECULAR WEIGHT

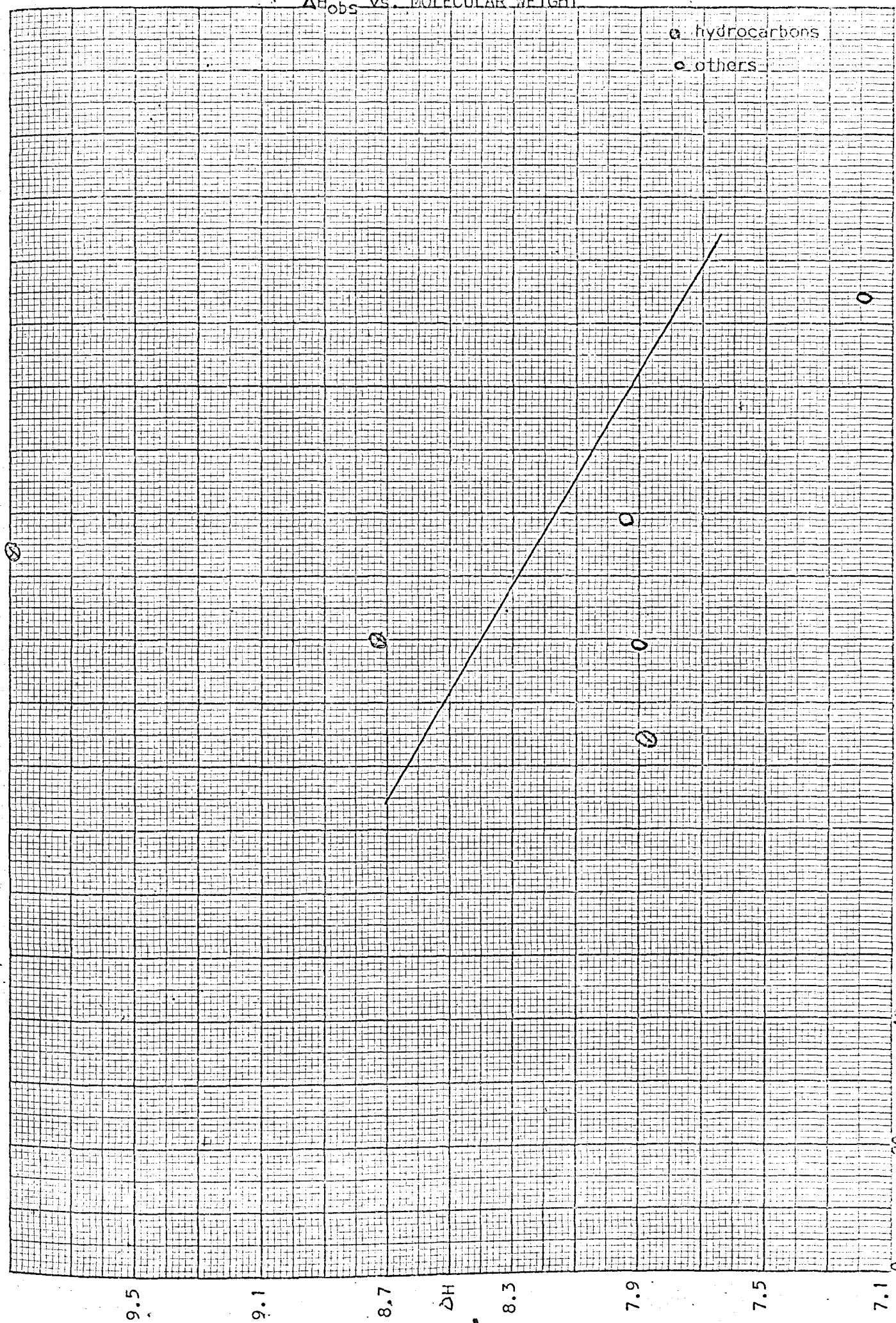


Figure 22
log(ΔH) vs. log(M)

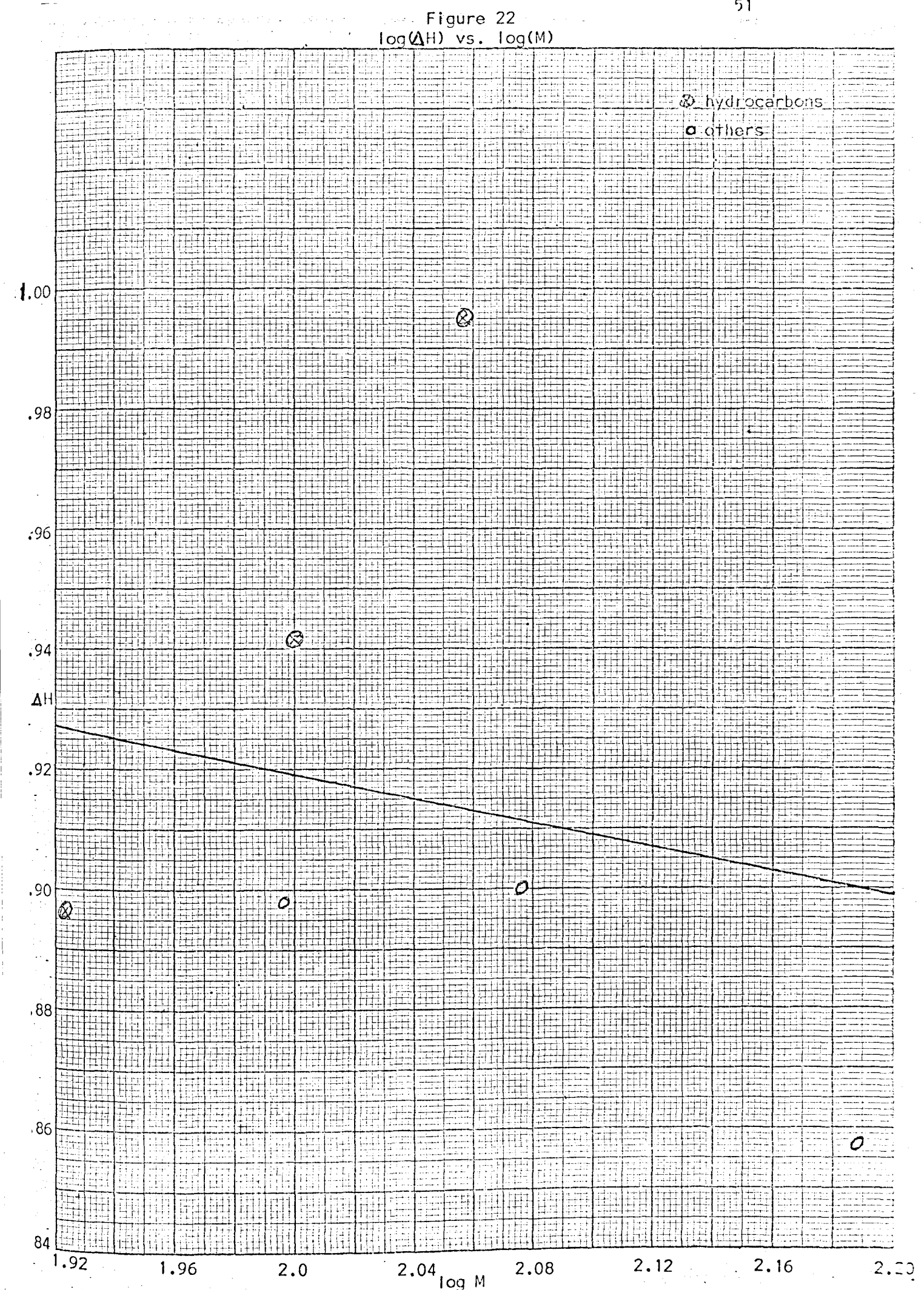


Table 6

ΔH for Homologous Series of Hydrocarbons

Hydrocarbon	M	ΔH Kcal/mole
Methane	16	2.03
Propane	44	4.48
Butane	58	5.34
Pentane	72	6.15
Hexane	86	6.72
Heptane	100	7.70

Source: Timmerman, J., Physico-Chemical Constants of Pure Organic Compounds, Elsevier Publishing Company (New York) 1950.

$$\log \Delta H = 0.719 \log M - 0.549 \qquad (64)$$

Converting equation (64) we have

$$\Delta H = 0.282\ M^{0.719} \qquad (65)$$

These fits are shown in Figures 23 and 24.

Standard Error is defined as

$$\sigma = \sqrt{\frac{(\Delta H_{obs} - \Delta H_{calc})^2}{n}} \qquad n = \#\ \text{of data points}$$

and has been calculated for each fit.

Table 7 summarizes Standard Error for the correlations developed here relating ΔH and ΔH^{o} to M as well as for those reference correlations mentioned in Section I which utilize molecular weight as an independent variable.

The accuracy of the correlations developed in this work fall short of that determined from Kuloor's equation applied to a homologous series of pure hydrocarbons. It is well, however, to note that Kuloor's equation requires the tabulation of values for C and n for every family of compounds considered while our correlations involving ΔH^{o} are based on a variety of compounds from different families with alcohols being the only exclusion. It is unfortunate that the limited amount of data available for this work prevented a more thorough study of the influence of family groupings on ΔH^{o}.

A promising note is the increase in accuracy of the correlations involving ΔH^{o} (equations (57) and (59)) over those involving ΔH (equations (60) and (62)). A 50% reduction in Standard Error certainly adds confidence to our hypothesis that a molecule in the infinitely dilute state in a non-polar solvent will demonstrate more regular behavior than when it is in the pure state.

Figure 23
Hydrocarbons ΔH vs. MOLECULAR WEIGHT

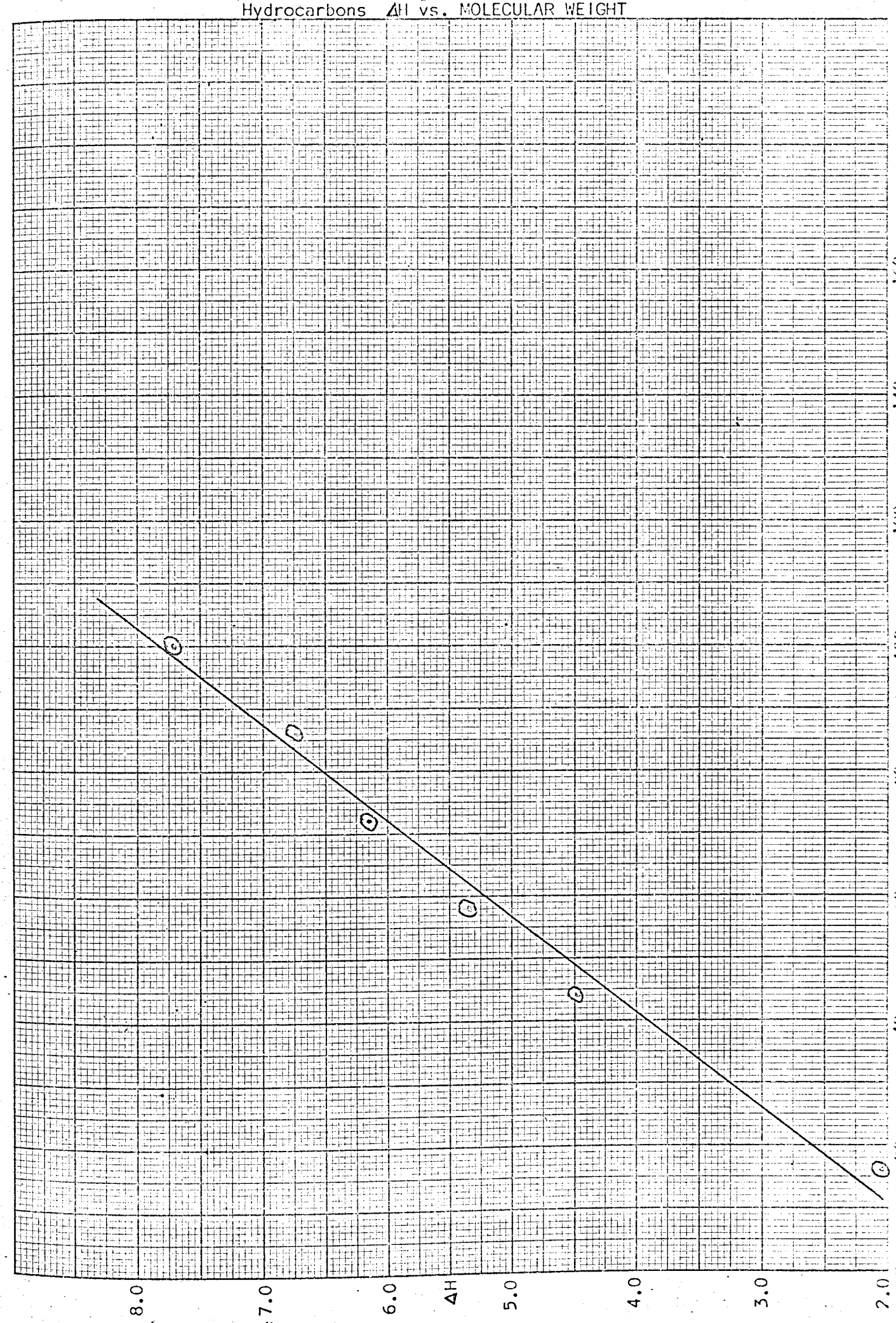


Figure 24

Hydrocarbons log ΔH vs. log M

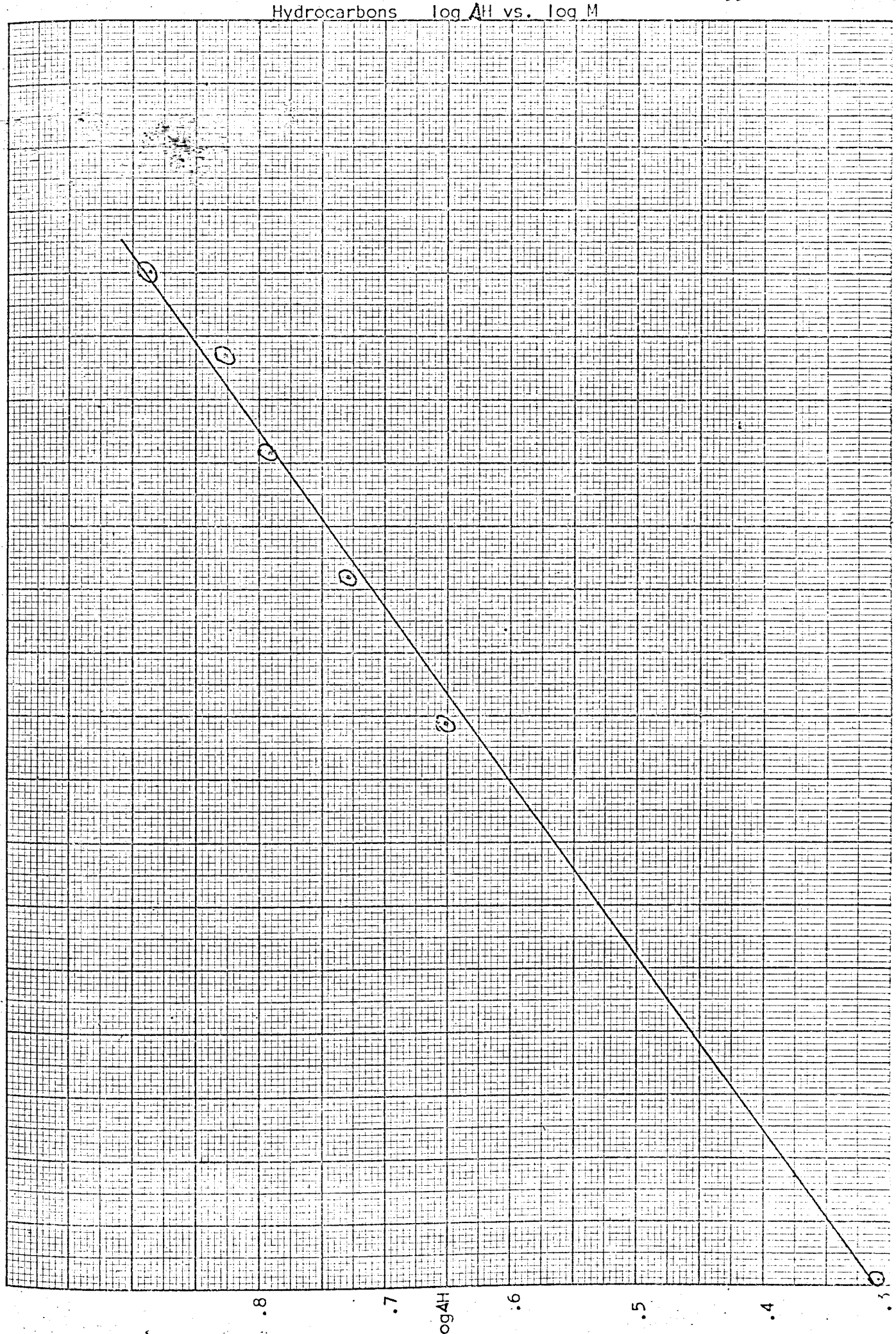


Table 7

Correlation	Equation #	Source	Standard Error
Hypothetical Heat of Vaporization			
$\Delta H^{\circ} = 0.0034\ M + 6.81$	(57)	___	0.42
$\Delta H^{\circ} = 6.08\ M^{0.0357}$	(59)	---	0.42
Standard Heat of Vaporization for pure substances (Same systems as correlated above)			
$\Delta H = -0.0116\ M + 9.55$	(60)	---	0.82
$\Delta H = 16.2\ M^{-0.145}$	(62)	---	0.84
Standard Heat of Vaporization for pure hydrocarbons			
$\Delta H = 0.0653\ M + 1.31$	(63)	---	0.24
$\Delta H = 0.282\ M^{0.719}$	(65)	---	0.16
Literature cited			
$\Delta H = CM^{-n}$ (cal/g)	(21)	Kuloor[16]	0.14 @ $\Delta H = 7.00$
$\Delta H = \sqrt[8]{\frac{L\ (D - d)}{M}}$	(24)	Wright[42]	not available
$\Delta H_v = m\left(\frac{\Delta H_{vw}\ \Delta Z}{\Delta Z_w}\right)_T$	(12)	Othmer[31] Fishtine[9]	0.56 @ $\Delta H = 7.00$

The correlations of ΔH to M exhibit negative slopes indicating an unexpected inverse relationship between the variables. The positive slope of the ΔH^{o} correlations to M show the expected relationship between the variables.

There is no significant difference between the accuracy of the linear correlation of ΔH^{o} (equation (57)) and that of the logarithmic correlation of ΔH^{o} (equation (59)) to molecular weight. However if ΔH^{o} is directly related to molecular weight, one would expect ΔH^{o} to approach zero as M approached zero. This is predicted only by the logarithmic correlation of equation (59).

VIII. SUMMARY

Beginning with the Clausius Clapeyron equation, correlations of pressure to temperature and heat of vaporization to molecular properties are reviewed.

All correlations of heat of vaporization to molecular properties are either limited in scope of application or too complicated to be easily handled without computer facilities.

The idealized heat of vaporization, ΔH°, is defined as being the heat of vaporization calculated from the Clausius-Clapeyron equation using a hypothetical vapor pressure which reflects the behavior of the component at infinite dilution in a non-polar solvent.

A method has been developed to obtain the limiting slope of a smooth curve through a series of experimental points, a problem frequently encountered.

Idealized heats of vaporization are calculated for compounds representing several chemical classes. With the exclusion of alcohols, the following linear and logarithmic correlations of ΔH° to molecular weight are shown to have a significantly lower Standard Error than similar correlations using standard heats of vaporization for the pure substances.

$$\Delta H^{\circ} = 0.0034\ M + 6.81$$

$$\Delta H^{\circ} = 6.08\ M^{0.0357}$$

Computer programs for conducting the necessary calculations and curve fitting are presented.

SYMBOLS

Unless otherwise noted in the text, the symbols used in this thesis are as follows:

a_n	- n^{th} coefficient of a power series
A_γ	- thermodynamic consistency constant
A,B,C,D,K	- constants
$\Delta H, \Delta H_v$	- heat of vaporization
ΔH^o	- idealized heat of vaporization
k_H	- Henry's law constant
M	- molecular weight
n	- carbon number
P	- vapor pressure of pure component
p^o	- hypothetical vapor pressure of pure component
p_{12}	- total vapor pressure of a binary system
p_2	- partial pressure of solute in a binary system
p_1	- partial pressure of solvent in a binary system
p_2^o	- hypothetical partial pressure of solute in a binary system
R	- gas law constant
T	- temperature
^oC	- degrees Centigrade
^oK	- degrees Kelvin
V	- volume
x_{2l}	- mole fraction solute in liquid
x_{2v}	- mole fraction solute in vapor
Z	- compressibility factor
γ_1	- activity coefficient of solvent
γ_2	- activity coefficient of solute
σ	- Standard Error

σ_{a_n} - standard error of the a_n coefficient of a power series

σ_{est} - standard error of the power series estimate

Subscripts

b - boiling point

c - critical variable

l - liquid

o - pure component

r - reduced

v - vapor

Superscript

o - idealized or hypothetical state

Appendix 1

Data

System: Methyl Alcohol/Benzene T= 35°C.

Reference: Scatchard G.,Wood S.E.,Mochel J.M.:J.Am.Chem.Soc. 68,1960(1946)

P_{12}	x_{2l}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
203.29	0.0242	0.2733	55.5592	11.0910	0.8053	1.1390
211.10	0.0254	0.3128	66.0321	12.5589	0.7917	1.2004
274.25	0.1302	0.4858	133.2306	4.9434	0.8624	0.7583
288.47	0.3107	0.5304	153.0045	2.3790	1.0454	0.3571
292.50	0.4989	0.5546	162.2205	1.5708	1.3829	0.0553
292.70	0.5191	0.5571	163.0632	1.5175	1.4339	0.0246
292.49	0.6305	0.5790	169.3517	1.2976	1.7726	-0.1355
283.58	0.7965	0.6421	182.0867	1.1044	2.6529	-0.3806
255.82	0.9197	0.7688	196.6744	1.0331	3.9179	-0.5789

PARTIAL PRESSURE CURVE FITTING:

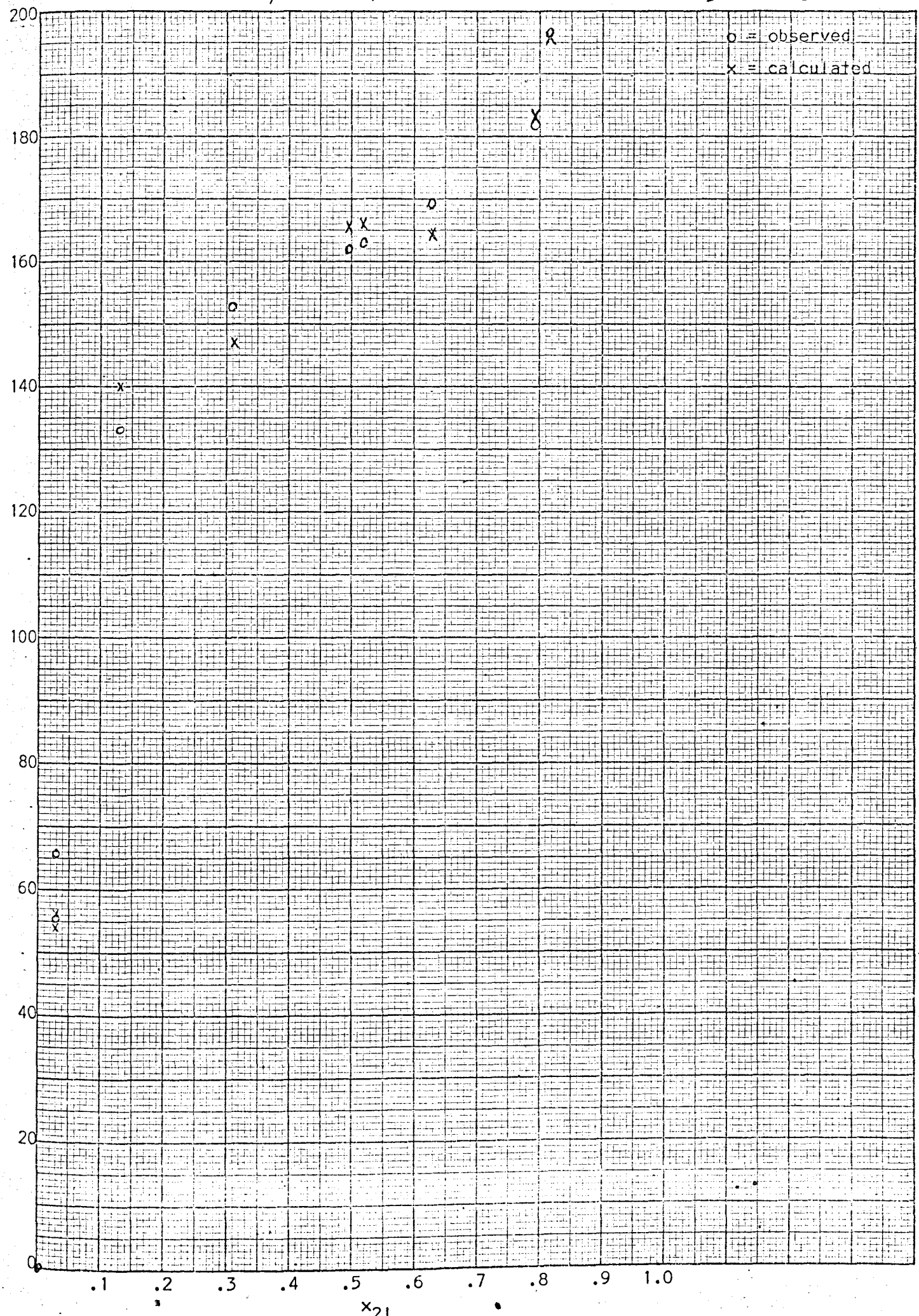
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	2654.8600	244.9079	10.8402	54.0680	1.4912
2	-18901.7789	3397.5342	-5.5634	56.2657	9.7664
3	65541.7388	16584.0780	3.9521	140.2284	-6.9977
4	-115711.4593	36206.0769	-3.1959	147.2542	5.7502
5	100068.6785	36168.7318	2.7667	165.6348	-3.4143
6	-33549.3841	13464.3511	-2.4917	166.1478	-3.0846
				164.5301	4.8217
				183.5524	-1.4657
				196.3783	0.2961

Degrees of Freedom= 4
Confidence in First Term= 99.5%+
Confidence in Last Term = 95.0%+

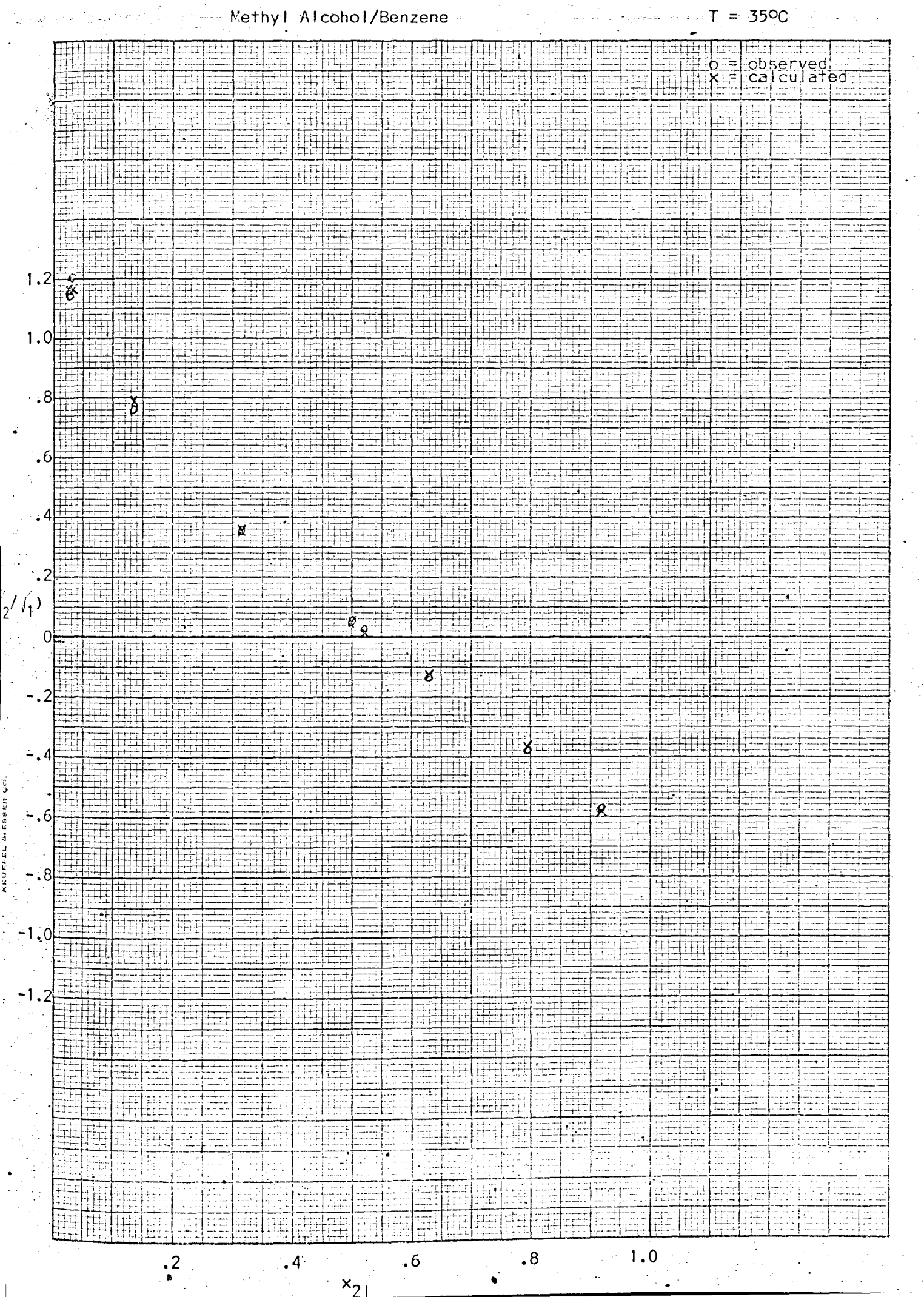
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$CAL.	DIF.
0	1.2618	0.0249	50.6378	1.1630	-0.0240
1	-4.1996	0.3219	-13.0471	1.1583	0.0421
2	4.8815	0.8615	5.6663	0.7918	-0.0335
3	-2.7228	0.6039	-4.5084	0.3466	0.0106
				0.0435	0.0118
				0.0163	0.0083
				-0.1279	-0.0076
				-0.3621	-0.0185
				-0.5897	0.0107

Degrees of Freedom= 5
Integral at X=1: 0.1085
Error in Integral: 0.0218


Methyl Alcohol/Benzene
T = 35°C
o = observed
x = calculated
200
180
160
140
120
100
80
60
40
20
0
.1
.2
.3
.4
.5
.6
.7
.8
.9
1.0
x_{21}

Methyl Alcohol/Benzene T = 35°C



System: Methyl Alchol/Benzene T= 40°C.

Reference: Lee S.C.; J. Phys. Chem. 35,3558(1931)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
349.00	0.1410	0.5070	176.9430	4.3348	0.6070	0.8538
356.60	0.2270	0.5270	187.9282	2.8597	0.6612	0.6360
362.50	0.3040	0.5310	192.4875	2.1872	0.7402	0.4705
364.20	0.4020	0.5400	196.6680	1.6819	0.8490	0.2990
365.60	0.4680	0.5430	198.5208	1.4652	0.9517	0.1874
366.00	0.5520	0.5480	200.5680	1.2551	1.1190	0.0498
366.20	0.6430	0.5660	207.2692	1.1135	1.3490	-0.0834
362.50	0.7020	0.5800	210.2500	1.0345	1.5482	-0.1751
357.50	0.7500	0.5780	206.6350	0.9517	1.8287	-0.2836
345.20	0.8340	0.6410	221.2732	0.9165	2.2623	-0.3924
334.00	0.8780	0.6700	223.7800	0.8804	2.7377	-0.4927
325.20	0.8960	0.7230	235.1196	0.9064	2.6247	-0.4618
322.50	0.9150	0.7530	242.8425	0.9168	2.8398	-0.4910

PARTIAL PRESSURE CURVE FITTING:

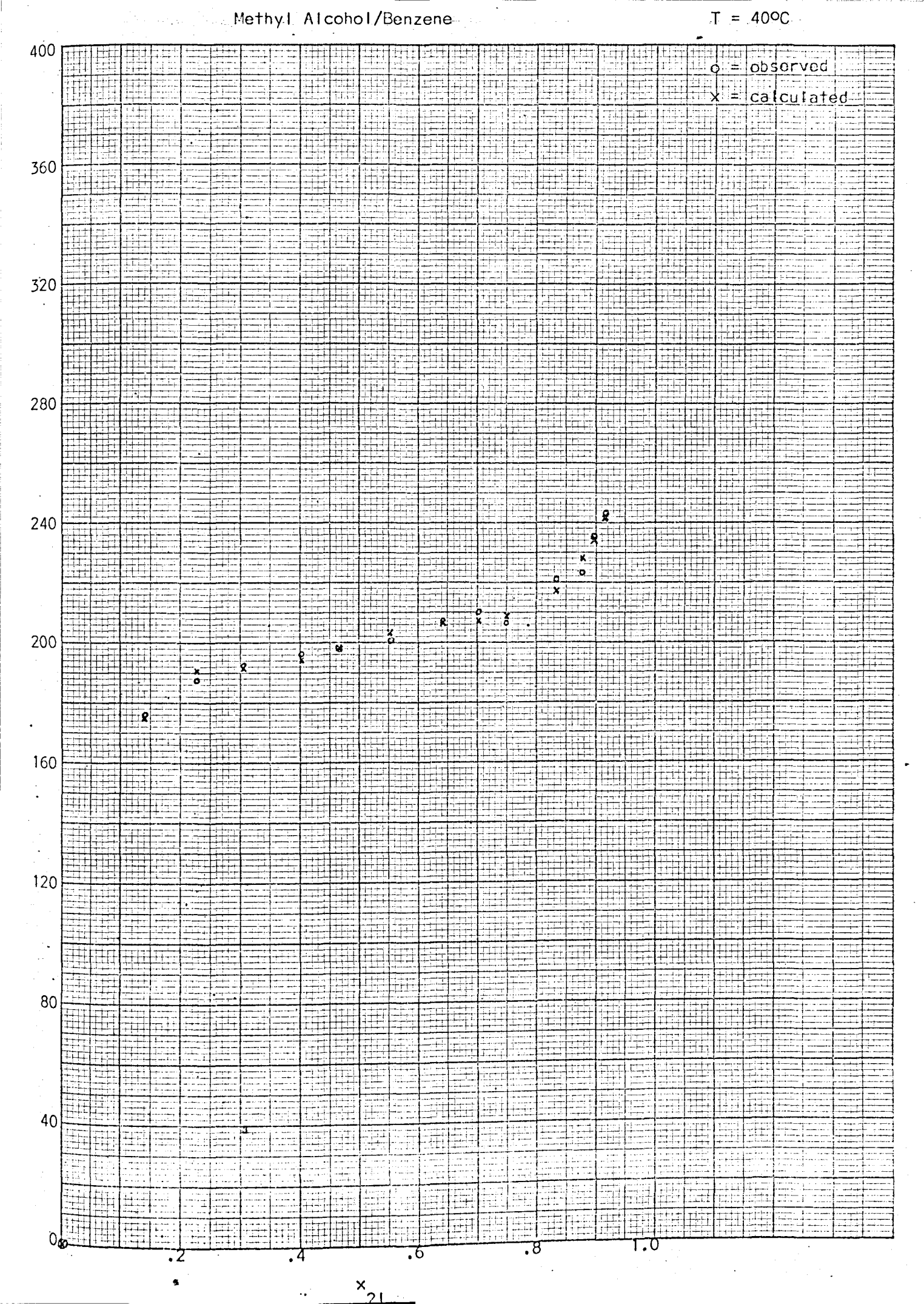
n	a_n	STD.ERROR	t
1	2591.0315	146.3411	17.7054
2	-13795.8824	1679.5115	-8.2142
3	36565.5446	7056.1939	5.1820
4	-50345.9008	13793.8218	-3.6419
5	34238.1899	12723.8860	2.6909
6	-8962.7804	4477.0599	-2.0019

Degrees of Freedom: 8
Confidence in First Term: 99.5%+
Confidence in Last Term: 95.0%+

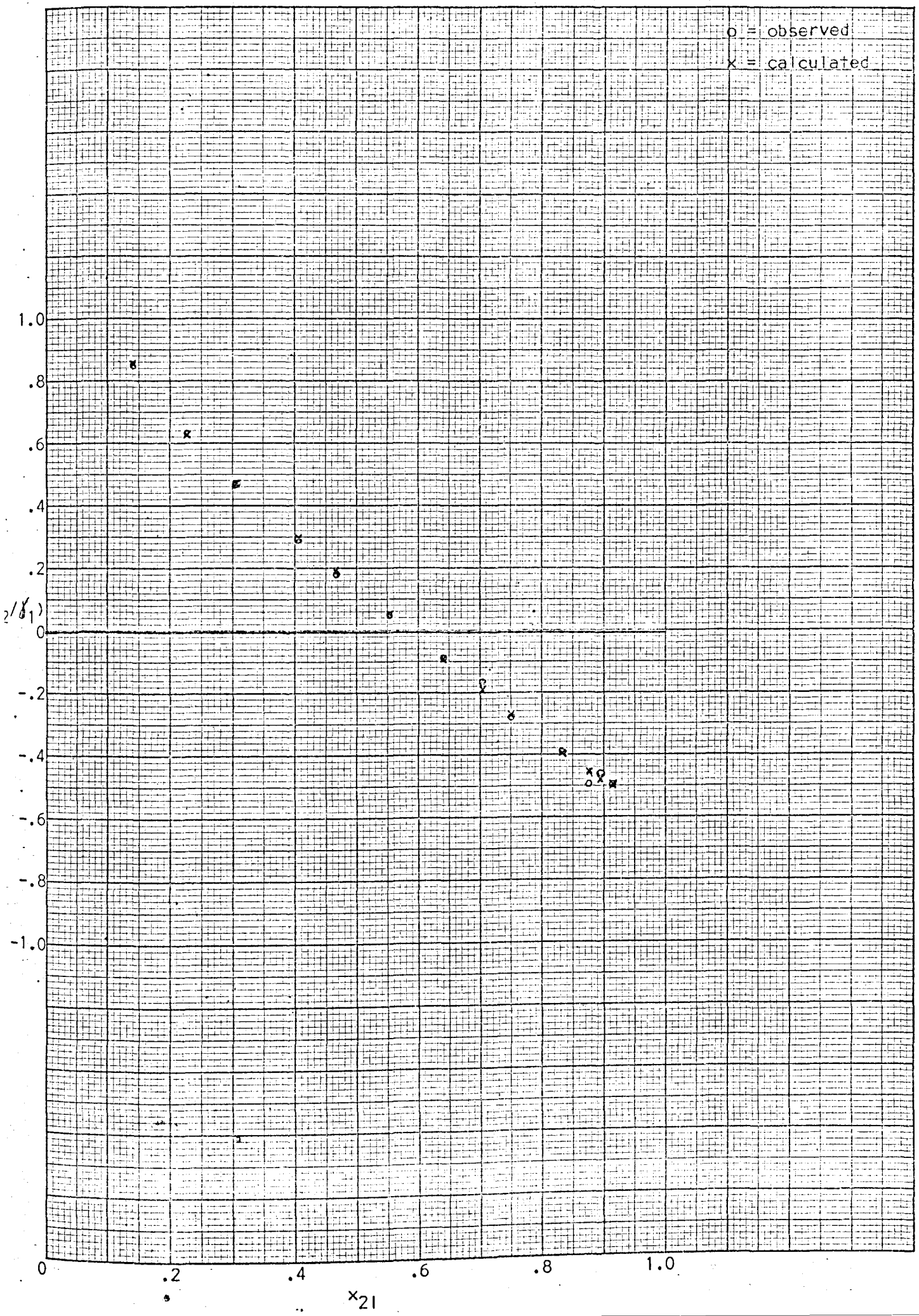
P_2 CALC.	DIF.
0.0000	0.0000
175.4991	1.4439
190.7164	-2.7882
191.8336	0.6539
194.3977	2.2703
198.3900	0.1308
203.6035	-3.0355
206.7015	0.5677
207.6582	2.5918
209.1218	-2.4868
217.9334	3.3398
228.3982	-4.6182
234.2725	0.8451
241.6129	1.2296

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$CAL.	DIF.
0	1.4254	0.1033	13.8046	0.8570	-0.0032
1	-5.2135	1.0766	-4.8428	0.6295	0.0064
2	9.9706	3.6594	2.7246	0.4702	0.0003
3	-11.9767	4.9701	-2.4097	0.2997	-0.0007
4	5.2405	2.3321	2.2472	0.1930	-0.0056
				0.0577	-0.0079
Degrees of Freedom: 8				-0.0927	0.0094
Integral at X=1: 0.1961				-0.1916	0.0165
Error in Integral: 0.0133				-0.2708	-0.0128
				-0.3998	0.0074
				-0.4579	-0.0348
				-0.4789	0.0171
				-0.4989	0.0079


Methyl Alcohol/Benzene
T = 40°C
o = observed
x = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x1

Methyl Alcohol/Benzene — T = 40°C



System: Methyl Alcohol/Benzene T= 55°C.

Reference: Scatchard G.,Wood S.E.,Mochel J.M.:J. Am. Chem. Soc. 68,1960(1946)

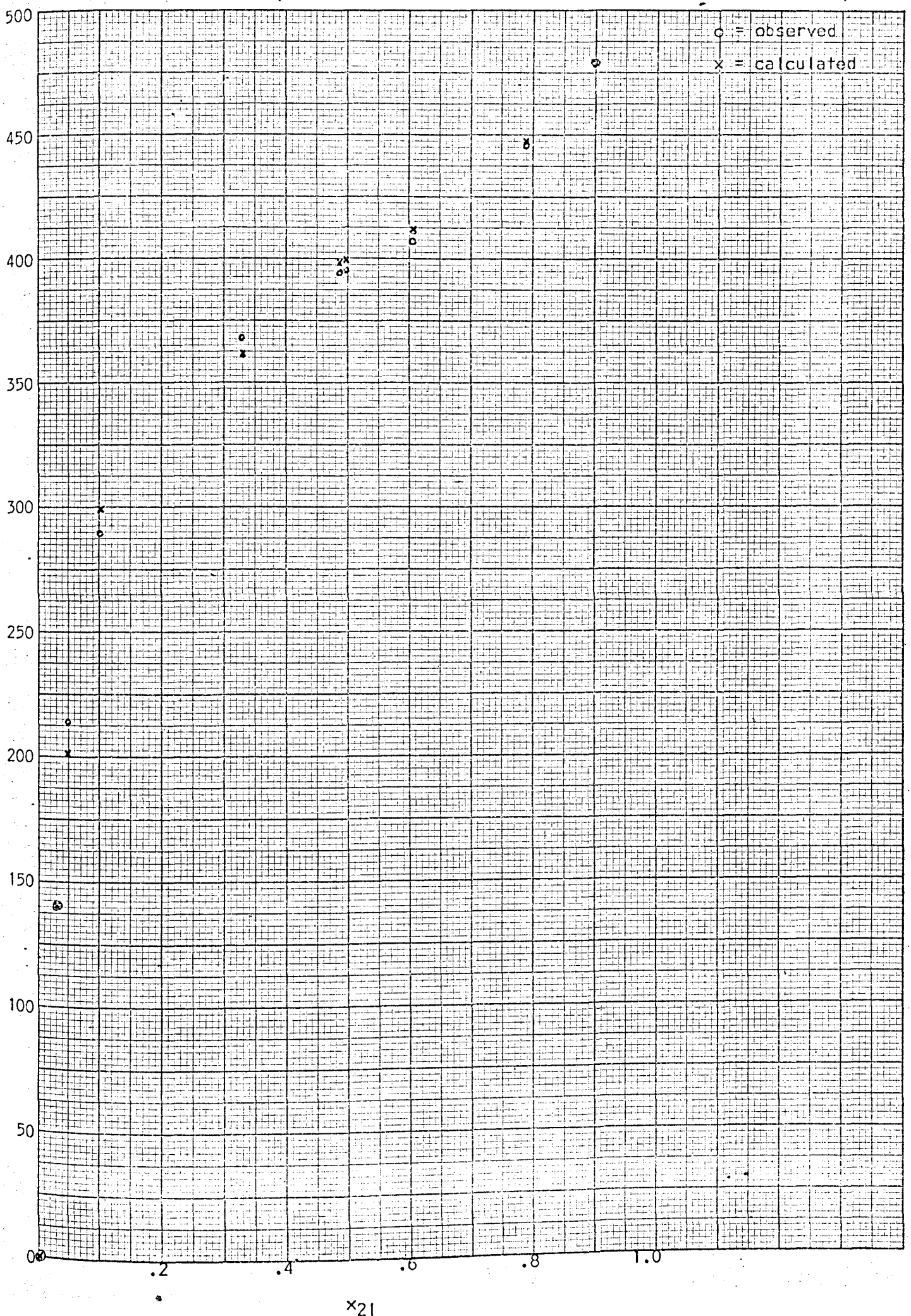
P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
465.84	0.0304	0.3019	140.6371	8.1162	0.7800	1.0173
527.12	0.0493	0.4051	213.5363	7.5989	0.7671	0.9959
597.48	0.1031	0.4841	289.2401	4.9218	0.7992	0.7894
664.24	0.3297	0.5540	367.9890	1.9581	1.0278	0.2799
675.62	0.4874	0.5845	394.8999	1.4214	1.2736	0.0477
675.99	0.4984	0.5858	395.9949	1.3939	1.2981	0.0309
678.44	0.6076	0.6078	412.3558	1.1906	1.5770	-0.1220
664.91	0.7896	0.6716	446.5536	0.9922	2.4135	-0.3861
622.29	0.9014	0.7697	478.9766	0.9322	3.3802	-0.5594

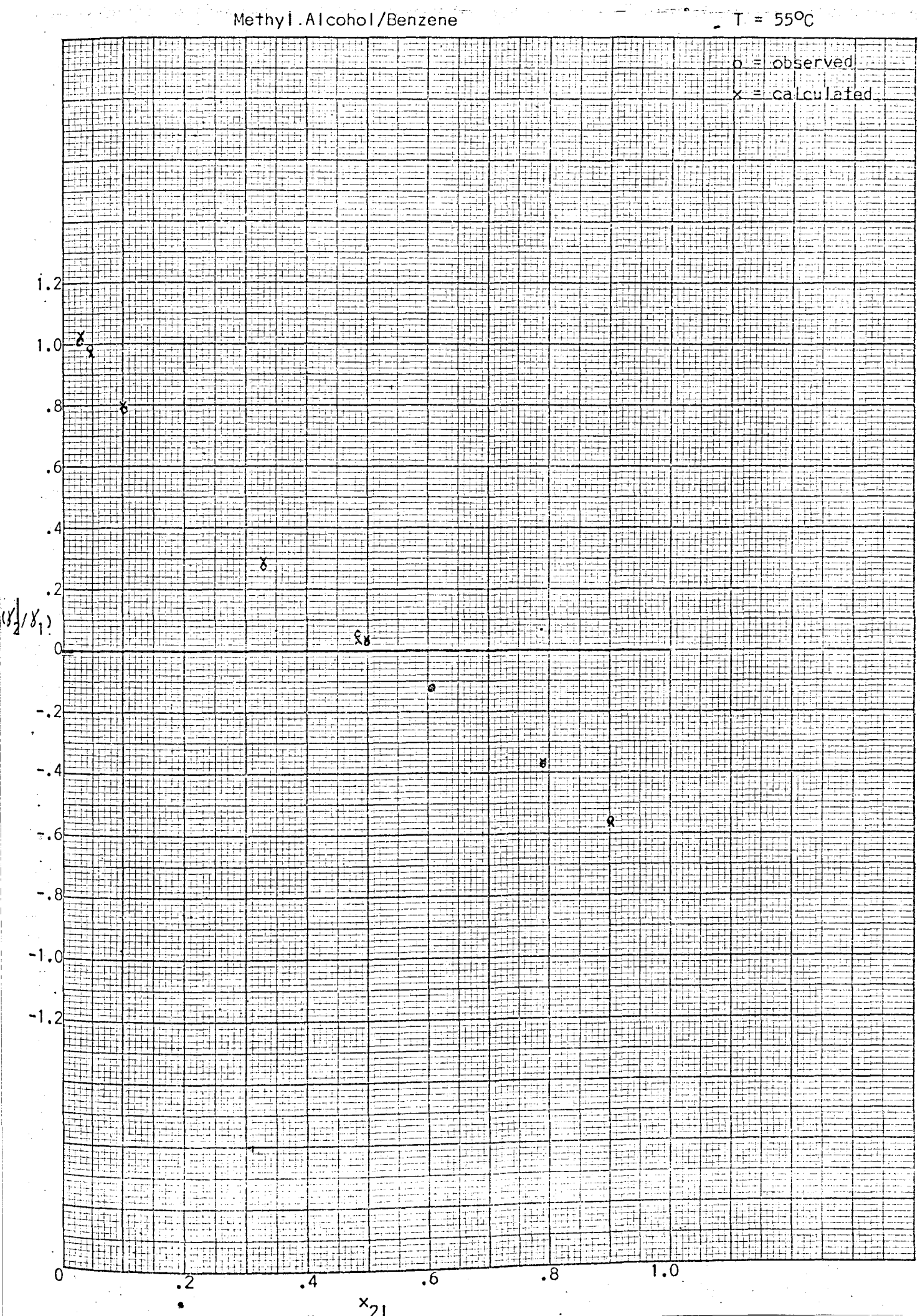
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	5636.3847	274.7139	20.5173	140.3618	0.2753
2	-37073.6786	4572.5972	-8.1078	201.2997	12.2366
3	122921.4285	23924.8828	5.1378	299.9109	-10.6709
4	-211109.6170	53908.7866	-3.9161	362.1779	5.8110
5	179572.7630	54867.4167	3.2728	398.4313	-3.5314
6	-59650.3935	20717.3253	-2.8793	399.9999	-4.0050
				407.3480	5.0078
Degrees of Freedom= 4				447.8602	-1.3066
Confidence in First Term= 99.5%+				478.6672	0.3094
Confidence in Last Term= 97.5%+					

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	SD.ERR.	t	$\log(\gamma_2/\gamma_1)$CAL.	DIF.
0	1.1378	0.0167	68.0293	1.0314	-0.0142
1	-3.6144	0.2280	-15.8542	0.9687	0.0272
2	3.8317	0.6155	6.2253	0.8036	-0.0141
3	-2.1280	0.4349	-4.8926	0.2864	-0.0065
				0.0400	0.0077
Degrees of Freedom= 5				0.0247	0.0062
Integral at x=1: 0.0759				-0.1210	-0.0010
Error in Integral: 0.0127				-0.3748	-0.0113
				-0.5654	0.0060


Methyl-Alcohol/Benzene
T = 55°C
o = observed
x = calculated
500
450
400
350
300
250
200
150
100
50
0
.2
.4
.6
.8
1.0
x_{21}


Methyl Alcohol/Benzene
T = 55°C
o = observed
x = calculated
1.2
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
-1.2
(γ_2/γ_1)
0
.2
.4
.6
.8
1.0
x_{21}

System: Ethyl Alcohol/Benzene T= 40°C.

Reference: Udovenko & Fatkoulina,1952: Physico-Chemical Constants of Binary Systems,Timmerman

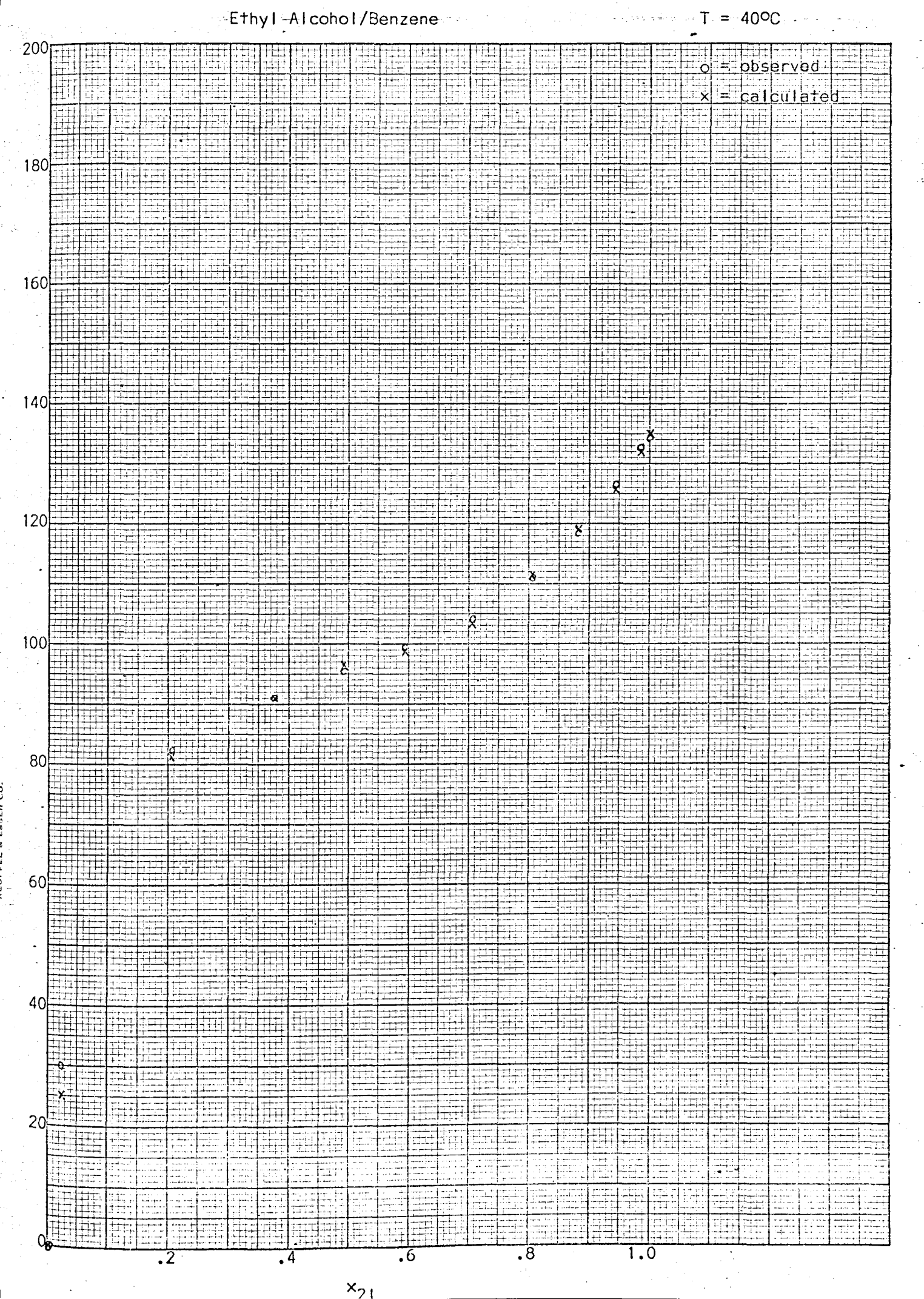
P_{12}	x_{2l}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
134.40	1.0000	1.0000	134.4000	1.0000	1.0000	0.0000
145.60	0.9870	0.9120	132.7872	1.0010	5.3624	-0.7289
169.50	0.9430	0.7470	126.6165	0.9990	4.0933	-0.6125
196.30	0.8800	0.6050	118.7615	1.0041	3.5155	-0.5442
219.40	0.8020	0.5070	111.2358	1.0320	2.9722	-0.4594
237.30	0.7020	0.4400	104.4120	1.1067	2.4262	-0.3409
245.70	0.5920	0.4050	99.5085	1.2507	1.9495	-0.1928
248.80	0.4900	0.3840	95.5392	1.4507	1.6350	-0.0519
252.30	0.3780	0.3620	91.3326	1.7978	1.4080	0.1061
249.10	0.2040	0.3320	82.7012	3.0164	1.1373	0.4236
239.80	0.0950	0.2800	67.1440	5.2588	1.0380	0.7047
208.40	0.0200	0.1450	30.2180	11.2418	0.9892	1.0555
183.80	0.0000	0.0000	0.0000	1.0000	1.0000	0.0000

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	1468.6718	107.0893	13.7145	135.0377	-0.6377
2	-11084.7136	1654.6900	-6.6990	132.3099	0.4773
3	43855.7280	9473.5445	4.6293	125.8343	0.7822
4	-95242.0861	26276.7303	-3.6246	119.4075	-0.6460
5	114606.6891	37924.3426	3.0220	111.8321	-0.5963
6	-71583.9321	27380.3142	-2.6144	103.5669	0.8451
7	18114.6805	7808.8263	2.3198	99.0660	0.4425
				96.6748	-1.1356
Degrees of Freedom= 7				91.1357	0.1969
Confidence in First Term= 99.5%+				81.2772	1.4240
Confidence in Last Term= 95.0%+				70.1630	-3.0191
				25.2755	4.9425
				0.0000	0.0000

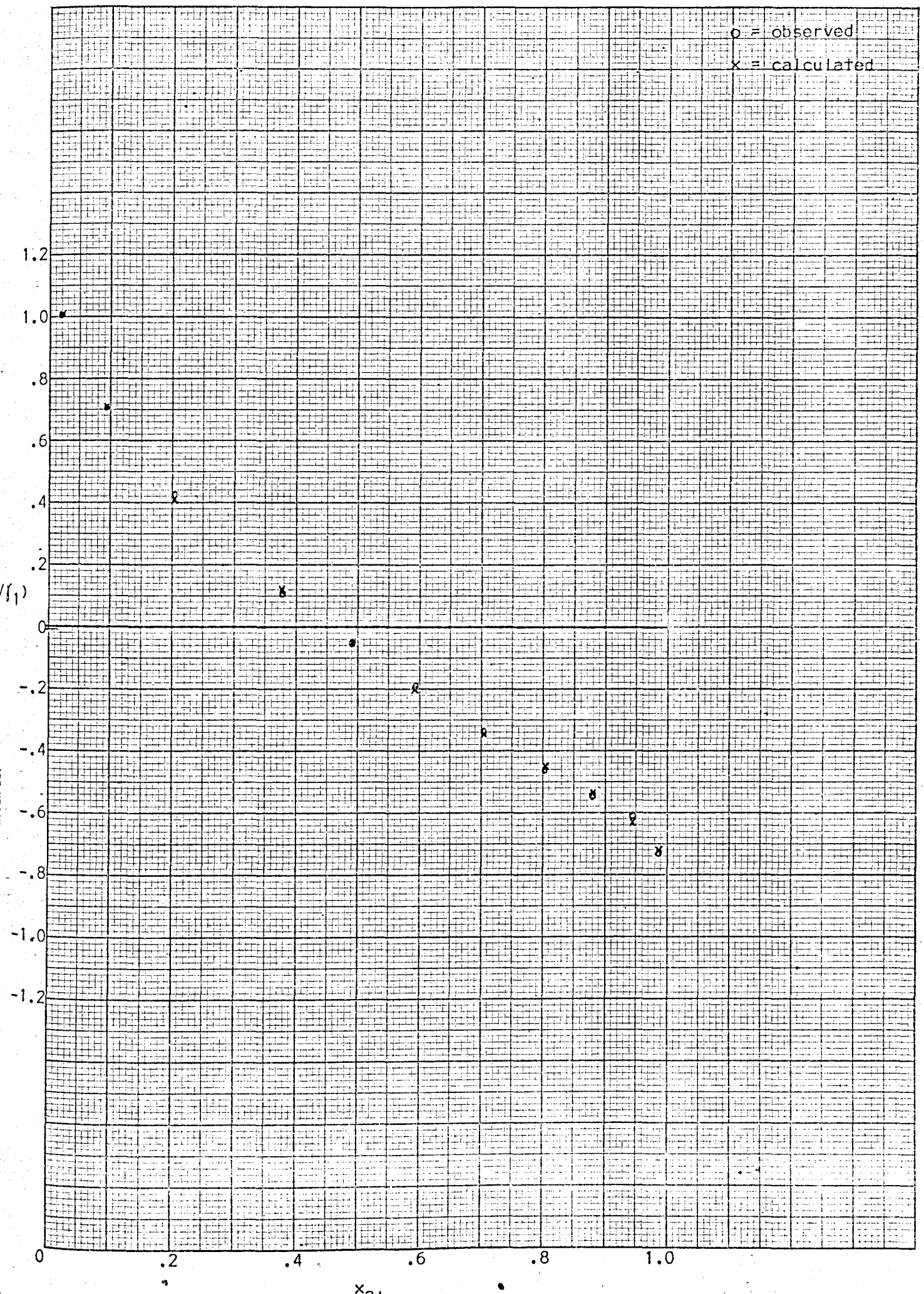
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.1747	0.0184	63.7518	-------	-------
1	-6.4329	0.4306	-14.9392	-0.7200	-0.0089
2	19.7708	2.8071	7.0431	-0.6306	0.0181
3	-39.1237	7.2412	-5.4029	-0.5384	-0.0058
4	37.6300	7.9840	4.7132	-0.4510	-0.0084
5	-13.7711	3.1496	-4.3723	-0.3419	0.0010
				-0.2012	0.0084
Degrees of Freedom= 5				-0.0530	0.0011
Integral at x=1: -0.0016				0.1169	-0.0108
Error in Integral: 0.0088				0.4134	0.0102
				0.7114	-0.0067
				1.0537	0.0019
				-------	-------


Ethyl-Alcohol/Benzene
T = 40°C
o = observed
x = calculated
200
180
160
140
120
100
80
60
40
20
0
.2
.4
.6
.8
1.0
x_{21}

Ethyl Alcohol/Benzene

T = 40°C



System: Ethyl Alcohol/Benzene T= 50°C.

Reference: Udovenko,Fatkoulina(1952):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{2l}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
222.60	1.0000	1.0000	222.6000	1.0000	1.0000	------
239.60	0.9840	0.9090	217.7964	0.9943	5.0174	-0.7029
276.80	0.9360	0.7450	206.2160	0.9897	4.0607	-0.6131
316.80	0.8660	0.6100	193.2480	1.0025	3.3948	-0.5297
344.40	0.7900	0.5260	181.1544	1.0301	2.8622	-0.4438
336.90	0.6940	0.4700	158.3430	1.0250	2.1485	-0.3214
378.10	0.5860	0.4340	164.0954	1.2580	1.9032	-0.1798
383.20	0.4860	0.4110	157.4952	1.4558	1.6168	-0.0455
384.60	0.3860	0.3920	150.7632	1.7546	1.4022	0.0974
378.30	0.2060	0.3600	136.1880	2.9699	1.1227	0.4225
358.70	0.0890	0.3000	107.6100	5.4317	1.0148	0.7286
314.70	0.0250	0.1650	51.9255	9.3307	0.9923	0.9733
271.60	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	2347.1665	149.5752	15.6922
2	-17558.3330	2349.1700	-7.4743
3	69874.0392	13672.2184	5.1107
4	-152793.3168	38424.3509	-3.9765
5	184120.0195	56018.5067	3.2868
6	-114395.9147	40756.7134	-2.8068
7	28628.6230	11693.5104	2.4482

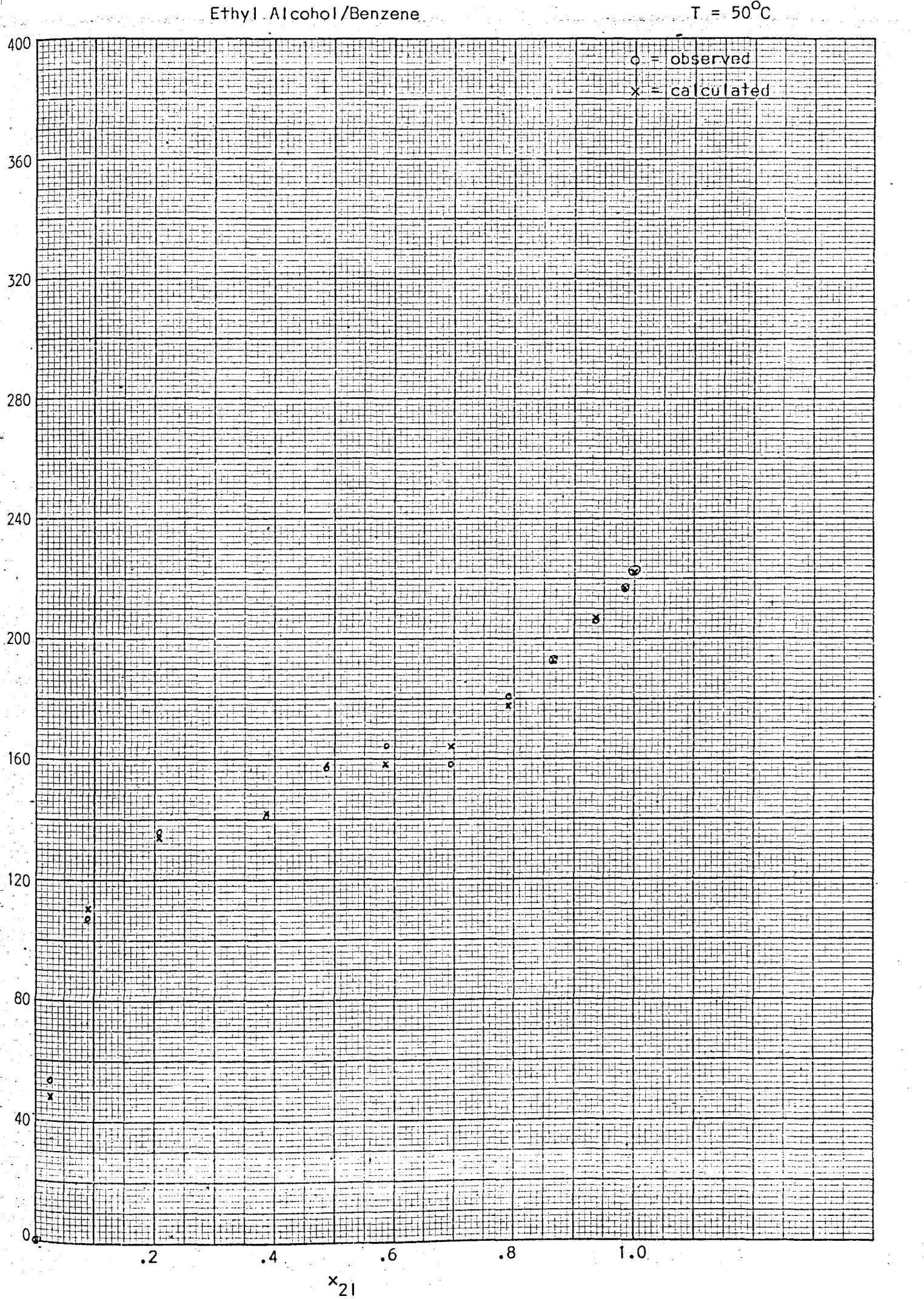
Degrees of Freedom= 6
Confidence in First Term= 99.5%+
Confidence in Last Term= 97.5%+

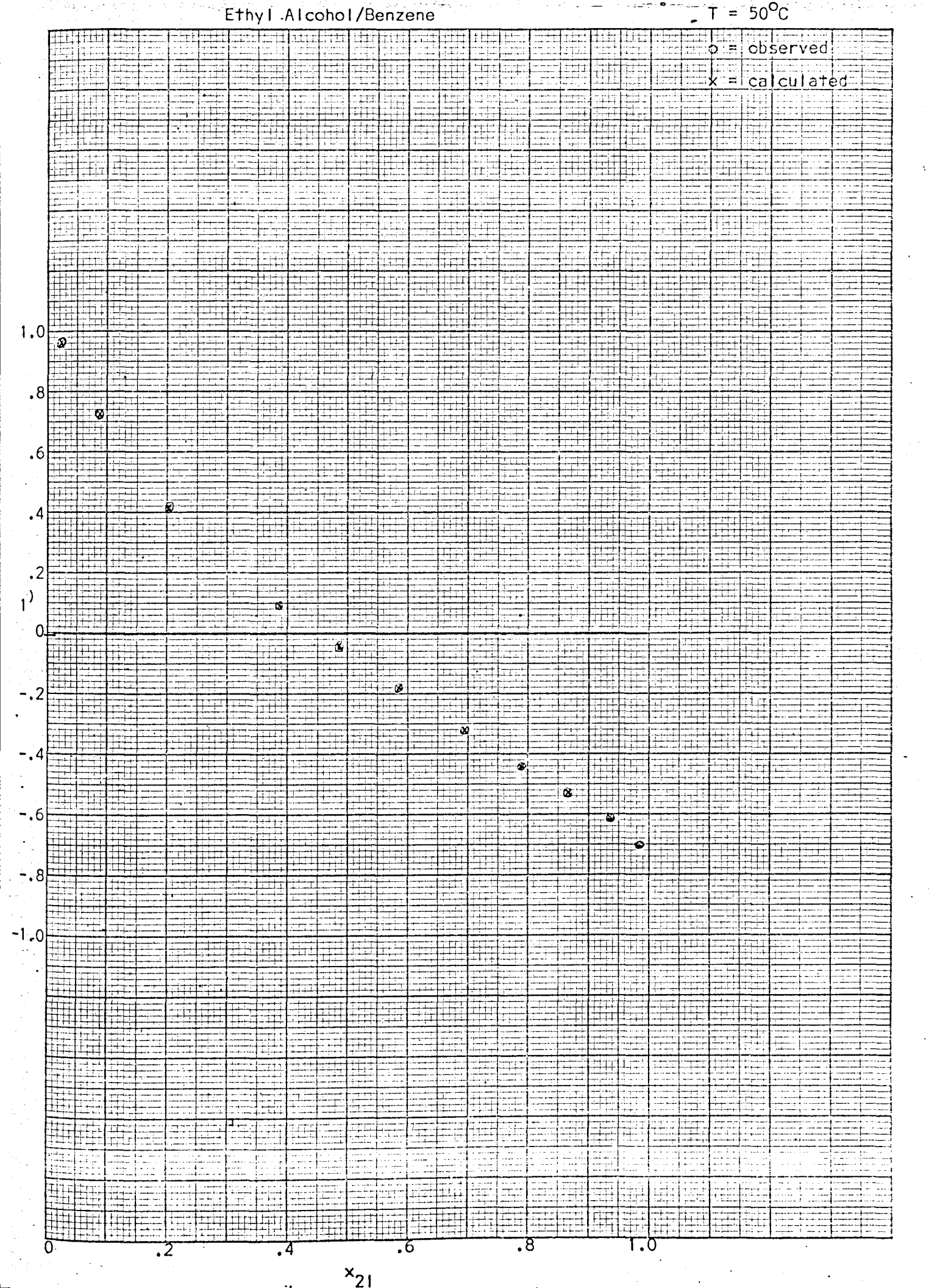
P_2 CALC.	DIF.
222.2836	0.3164
217.8128	-0.0164
207.1798	-0.9638
193.1442	0.1038
177.9829	3.1715
164.1393	-5.7963
159.2498	4.8456
158.3555	-0.8683
152.4445	-1.6813
134.0957	2.0923
110.4633	-2.8533
48.7391	3.1864
0.0000	0.0000

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.0988	0.0036	304.3808	------	------
1	-5.4706	0.1422	-38.4616	-0.7026	-0.0004
2	19.7465	1.6398	12.0418	-0.6142	0.0011
3	-69.8244	8.3042	-8.4083	-0.5287	-0.0011
4	164.5393	21.5812	7.6242	-0.4435	-0.0003
5	-228.6182	30.0087	-7.6184	-0.3229	0.0015
6	166.9273	21.2071	7.8713	-0.1787	-0.0011
7	-49.1425	5.9789	-8.2193	-0.0453	-0.0002
				0.0967	0.0007
				0.4229	-0.0005
				0.7283	0.0003
				0.9734	-0.0001

Degrees of Freedom= 3
Integral at x=1: -0.0016
Error in Integral: 0.0008


Ethyl Alcohol/Benzene
T = 50°C
o = observed
x = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x_{21}


Ethyl Alcohol/Benzene
T = 50°C
o = observed
x = calculated
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
0
.2
.4
.6
.8
1.0
x21

System: Ethyl Alcohol/Cyclohexane T= 10°C.

Reference: Nagai J.,Isii N.:J. Soc. Chem. Ind. Japan 38,86(1935

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
40.15	0.9500	0.5617	22.5523	0.7966	5.9452	-0.8729
50.65	0.9000	0.4294	21.7491	0.8109	4.8819	-0.7796
55.70	0.8500	0.3806	21.1994	0.8369	3.8852	-0.6667
58.60	0.8000	0.3532	20.6975	0.8682	3.2012	-0.5667
60.45	0.7500	0.3383	20.4502	0.9150	2.7027	-0.4704
61.80	0.7000	0.3261	20.1530	0.9661	2.3450	-0.3851
62.70	0.6500	0.3158	19.8007	1.0222	2.0704	-0.3065
63.30	0.6000	0.3089	19.5534	1.0936	1.8474	-0.2277
63.75	0.5500	0.3051	19.4501	1.1867	1.6629	-0.1465
64.15	0.5000	0.3017	19.3541	1.2989	1.5134	-0.0664
64.50	0.4500	0.2993	19.3048	1.4396	1.3881	0.0158
64.75	0.4000	0.2972	19.2437	1.6144	1.2811	0.1004
64.95	0.3500	0.2964	19.2512	1.8458	1.1876	0.1915
65.10	0.3000	0.2964	19.2956	2.1583	1.1053	0.2906
65.10	0.2500	0.2957	19.2501	2.5839	1.0327	0.3983
65.00	0.2000	0.2939	19.1035	3.2053	0.9691	0.5195
64.65	0.1500	0.2901	18.7550	4.1957	0.9121	0.6628
63.70	0.1000	0.2779	17.7022	5.9403	0.8633	0.8376
61.65	0.0500	0.2498	15.4002	10.3357	0.8224	1.0993

PARTIAL PRESSURE CURVE FITTING:

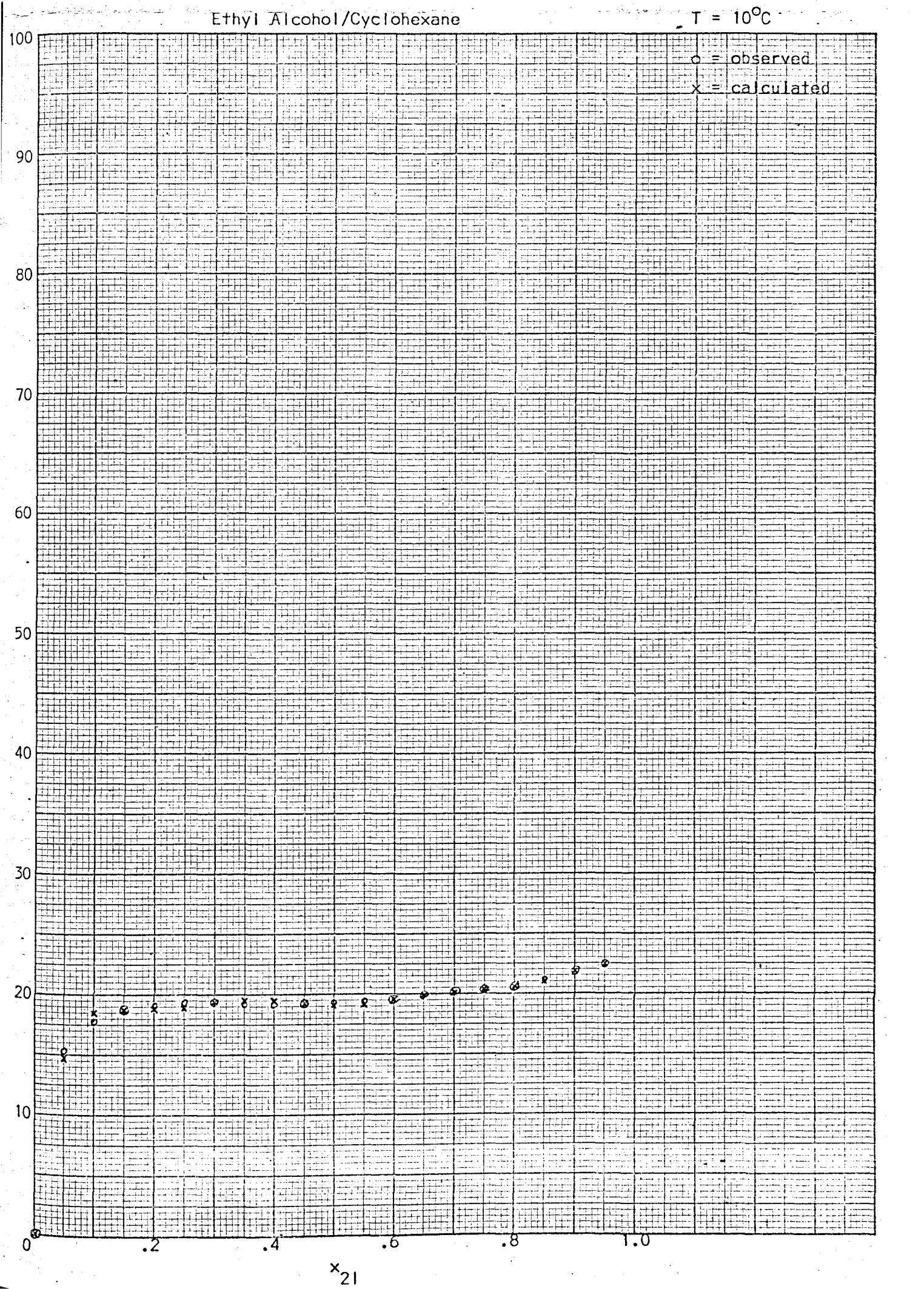
n	a_n	STD.ERROR	†
1	496.6101	18.3510	27.0617
2	-5255.2389	380.3124	-13.8182
3	28902.7901	3006.9248	9.6121
4	-90521.4071	11937.2526	-7.5831
5	167095.4351	26168.3037	6.3854
6	-179592.2615	32142.6669	-5.5873
7	103834.2357	20716.0236	5.0133
8	-24941.1717	5451.9739	-4.5747

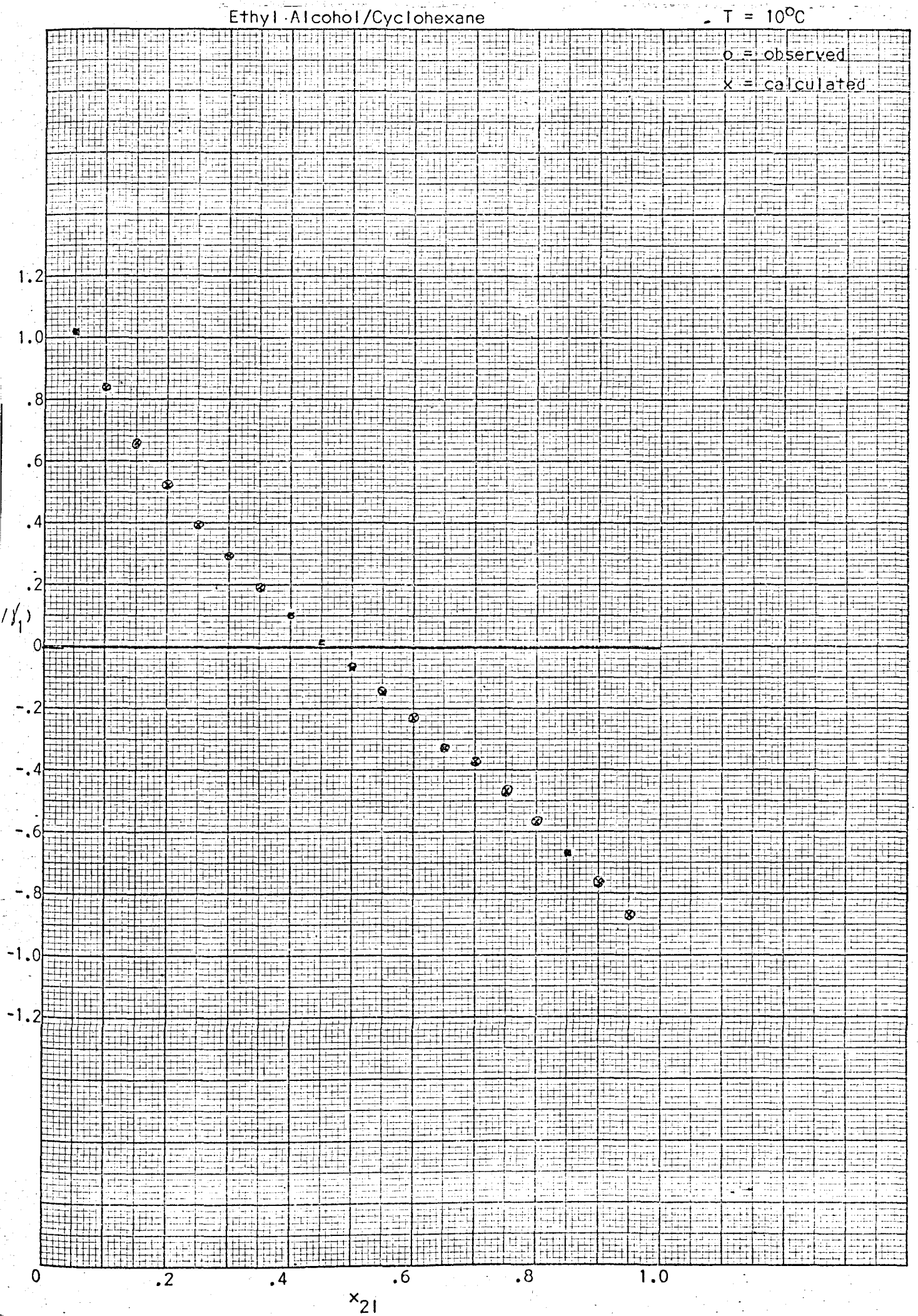
Degrees of Freedom= 12
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

P_2 CALC.	DIF.
22.4883	0.0640
21.9733	-0.2242
21.0360	0.1634
20.5770	0.1205
20.4412	0.0091
20.2939	-0.1409
19.9809	-0.1802
19.5710	-0.0176
19.2430	0.2071
19.1379	0.2161
19.2586	0.0463
19.4603	-0.2166
19.5351	-0.2839
19.3548	-0.0591
18.9973	0.2528
18.7424	0.3611
18.7832	-0.0283
18.4608	-0.7585
14.7890	0.6112

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.4621	0.0112	130.8456	-0.8739	0.0010
1	-8.7569	0.2669	-32.8058	-0.7760	-0.0036
2	33.3677	2.1087	15.8238	-0.6699	0.0032
3	-89.1263	7.5208	-11.8506	-0.5668	0.0001
4	135.0549	13.3377	10.1258	-0.4715	0.0011
5	-105.9340	11.4729	-9.2334	-0.3844	-0.0007
6	32.9891	3.8135	8.6506	-0.3036	-0.0029
				-0.2261	-0.0016
Degrees of Freedom= 12				-0.1488	0.0023
Integral at x=1: -0.0073				-0.0692	0.0029
Error in Integral: 0.0026				0.0141	0.0017
				0.1019	-0.0015
				0.1944	-0.0029
				0.2923	-0.0017
				0.3980	0.0004
				0.5168	0.0027
				0.6593	0.0035
				0.8435	-0.0058
				1.0974	0.0019


Ethyl Alcohol/Cyclohexane
T = 10°C
o = observed
x = calculated
100
90
80
70
60
50
40
30
20
10
0
.2
.4
.6
.8
1.0
x21


Ethyl Alcohol/Cyclohexane
T = 10°C
o = observed
x = calculated
1.2
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
-1.2
$\ln(\gamma_1)$
0
.2
.4
.6
.8
1.0
x_{21}

System: Ethyl alcohol/Cyclohexane T= 20°C.

Reference: Nagai J.,Isii N.:J. Soc. Chem. Ind. Japan 38,86(1935)

p_{12}	x_{2l}	x_{2v}	p_2	f_2	γ_1	$\log(\gamma_2/\gamma_1)$
70.95	0.9500	0.5983	42.4494	0.7979	5.6493	-0.8500
85.75	0.9000	0.4752	40.7484	0.8085	4.4600	-0.7417
94.25	0.8500	0.4196	39.5473	0.8308	3.6143	-0.6385
99.85	0.8000	0.3871	38.6519	0.8628	3.0326	-0.5459
103.40	0.7500	0.3675	37.9995	0.9047	2.5927	-0.4572
105.70	0.7000	0.3510	37.1007	0.9464	2.2662	-0.3792
107.20	0.6500	0.3424	36.7053	1.0084	1.9962	-0.2966
108.10	0.6000	0.3359	36.3108	1.0807	1.7787	-0.2164
108.70	0.5500	0.3312	36.0014	1.1689	1.6011	-0.1367
109.00	0.5000	0.3276	35.7084	1.2753	1.4528	-0.0566
109.20	0.4500	0.3269	35.6975	1.4166	1.3245	0.0292
109.40	0.4000	0.3264	35.7082	1.5941	1.2172	0.1171
109.50	0.3500	0.3261	35.7079	1.8218	1.1251	0.2093
109.60	0.3000	0.3258	35.7077	2.1255	1.0462	0.3078
109.70	0.2500	0.3237	35.5099	2.5364	0.9804	0.4128
109.60	0.2000	0.3230	35.4008	3.1608	0.9192	0.5364
109.30	0.1500	0.3194	34.9104	4.1560	0.8674	0.6805
107.90	0.1000	0.3068	33.1037	5.9114	0.8237	0.8559
104.50	0.0500	0.2776	29.0092	10.3604	0.7876	1.1191

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	823.7858	37.3349	22.0648
2	-7236.4059	600.9644	-12.0413
3	31430.0410	3622.6769	8.6759
4	-74163.7218	10600.6020	-6.9962
5	96689.6359	16150.1594	5.9869
6	-65369.0830	12314.6193	-5.3083
7	17879.8897	3710.9438	4.8102

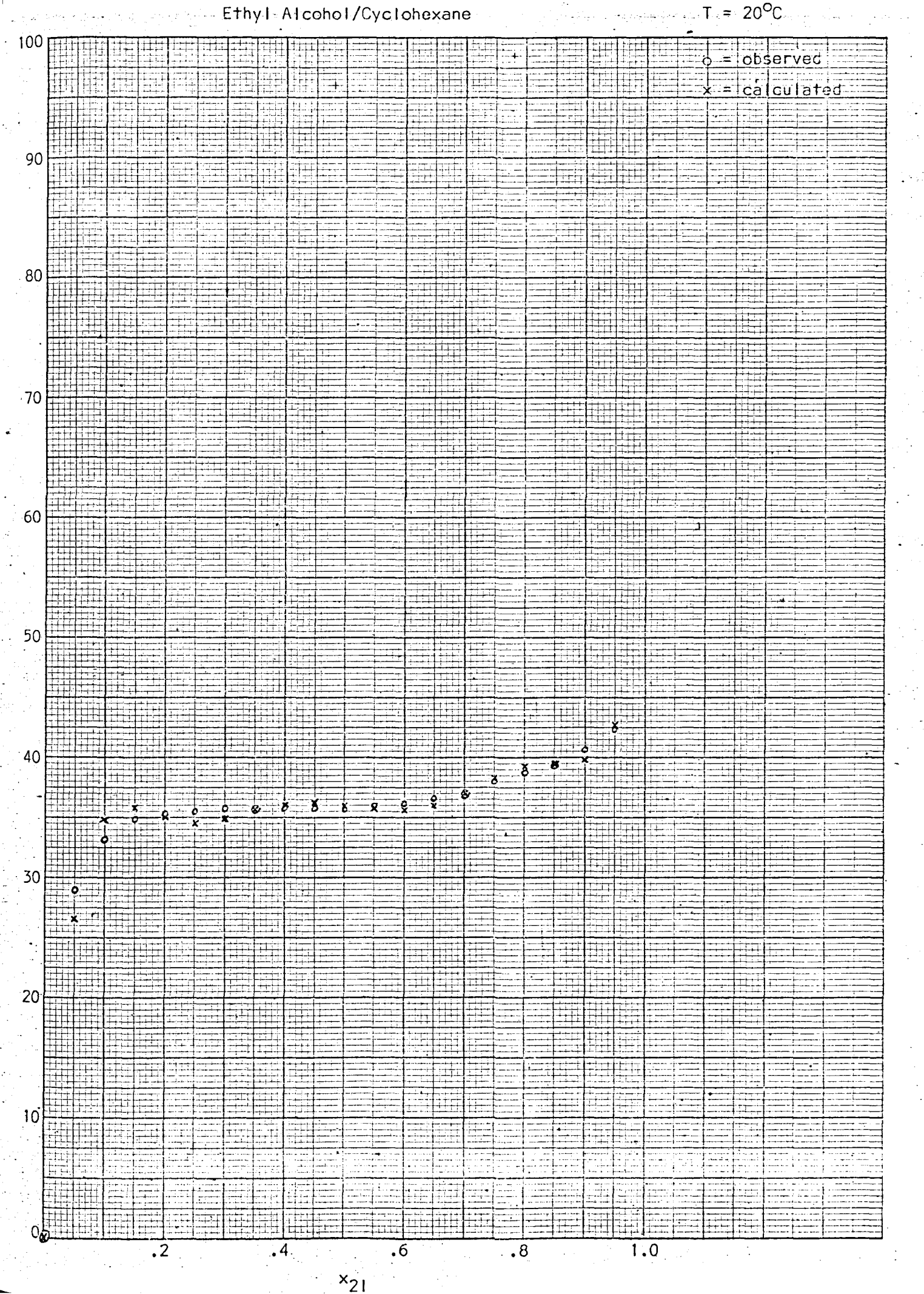
Degrees of Freedom= 13
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

p_2 CALC.	DIF.
42.7649	-0.3155
39.9486	0.7998
39.6324	-0.0851
39.2811	-0.6291
38.3331	-0.3336
37.1113	-0.0106
36.1235	0.5818
35.6845	0.6263
35.7884	0.2131
36.1598	-0.4514
36.4156	-0.7182
36.2652	-0.5571
35.6791	0.0288
34.9563	0.7514
34.6190	0.8909
35.0652	0.3356
35.9081	-0.9976
34.9315	-1.8278
26.5927	2.4165

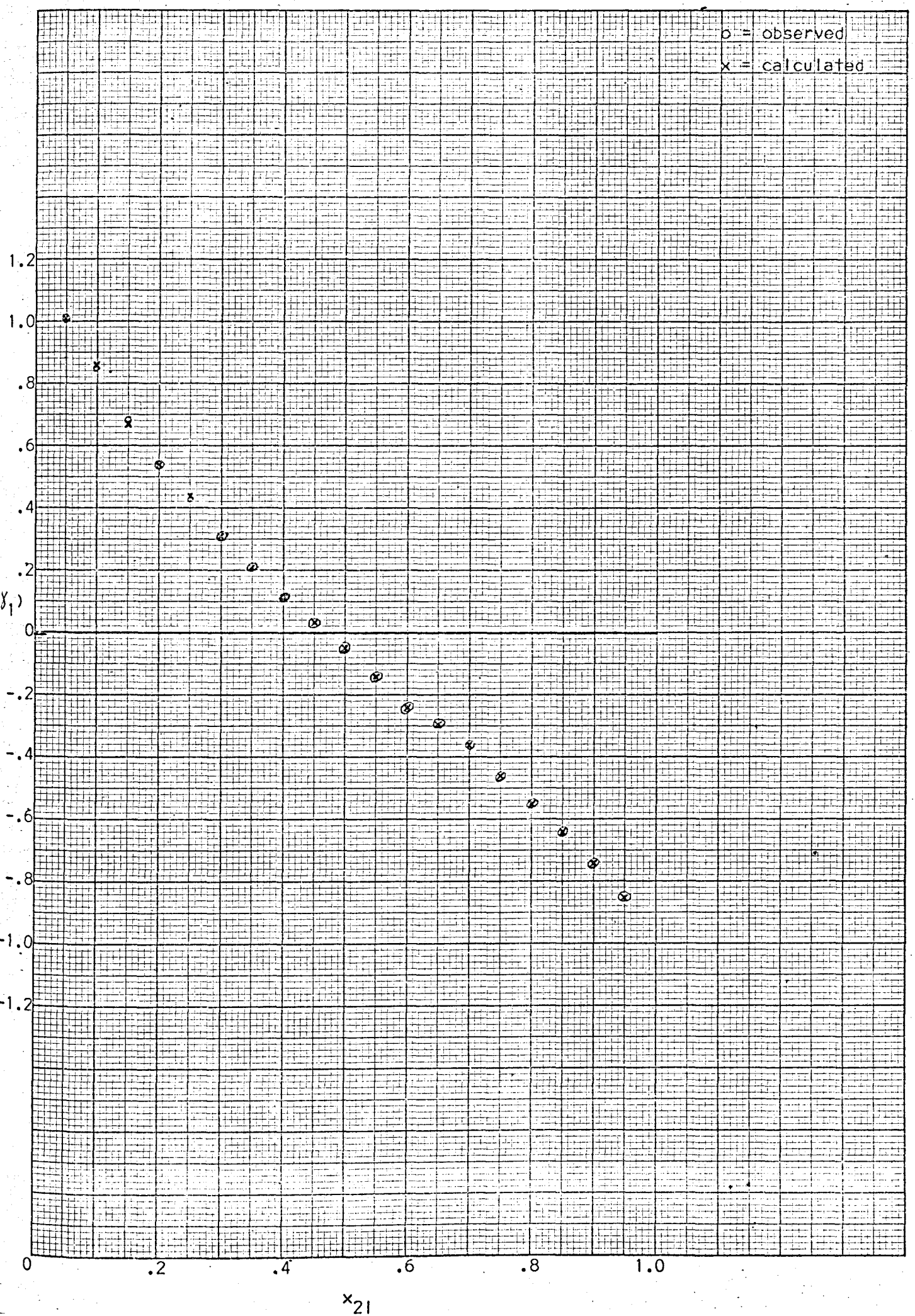
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.5392	0.0174	88.5126	-0.8499	-0.0001
1	-10.8307	0.6063	-17.8637	-0.7420	0.0003
2	59.1568	7.5014	7.8861	-0.6385	0.0000
3	-244.8843	45.3713	-5.3973	-0.5448	-0.0011
4	651.0510	152.0430	4.2820	-0.4590	0.0018
5	-1090.0464	296.2490	-3.6795	-0.3775	-0.0018
6	1106.3112	333.6001	3.3163	-0.2974	0.0008
7	-619.8866	201.1273	-3.0821	-0.2173	0.0009
8	146.6496	50.2088	2.9208	-0.1365	-0.0001
				-0.0547	-0.0019
				0.0291	0.0001
				0.1161	0.0010
				0.2083	0.0010
				0.3074	0.0004
				0.4156	-0.0028
				0.5363	0.0000
				0.6775	0.0030
				0.8580	-0.0021
				1.1187	0.0004

Degrees of Freedom= 10
Integral at x=1: 0.0105
Error in Integral: 0.0014


Ethyl Alcohol/Cyclohexane
T = 20°C
○ = observed
× = calculated
100
90
80
70
60
50
40
30
20
10
0
.2
.4
.6
.8
1.0
x21

Ethyl Alcohol/Cyclohexane T = 20°C



System: Ethyl Alcohol/Cyclohexane T= 25°C.

Reference: Washburn E.R.,Handorf B.H.:J. Am. Chem. Soc. 57,441(1935)

p_{12}	x_{21}	x_{2v}	p_2	f_2	f_1	$\log(f_2/f_1)$
108.40	0.8992	0.4796	51.9886	0.6661	4.3383	-0.8138
125.60	0.7948	0.3696	46.4218	0.6729	2.9912	-0.6479
132.60	0.7098	0.3532	46.8343	0.7602	2.2910	-0.4791
137.90	0.5941	0.3510	48.4029	0.9386	1.7092	-0.2603
139.40	0.4983	0.3424	47.7306	1.1035	1.4164	-0.1084
138.90	0.4016	0.3368	46.7815	1.3420	1.1933	0.0510
139.10	0.2987	0.3313	46.0838	1.7774	1.0282	0.2377
140.50	0.2050	0.3268	45.9154	2.5804	0.9223	0.4468
136.90	0.1030	0.3105	42.5074	4.7545	0.8157	0.7656

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	860.0895	26.7599	32.1410	52.0002	-0.0115
2	-6357.0776	455.5515	-13.9547	46.3255	0.0963
3	24182.9929	2882.0688	8.3908	47.0613	-0.2269
4	-51753.5723	8857.5474	-5.8429	48.0747	0.3282
5	63434.3311	14201.3652	4.4668	47.9499	-0.2194
6	-41842.1819	11414.8526	-3.6656	46.8798	-0.0983
7	11567.5085	3629.6100	3.1870	45.7941	0.2897
				46.1366	-0.2212
				42.4343	0.0731

Degrees of Freedom= 3
Confidence in First Term= 99.5%+
Confidence in Last Term= 97.5%+

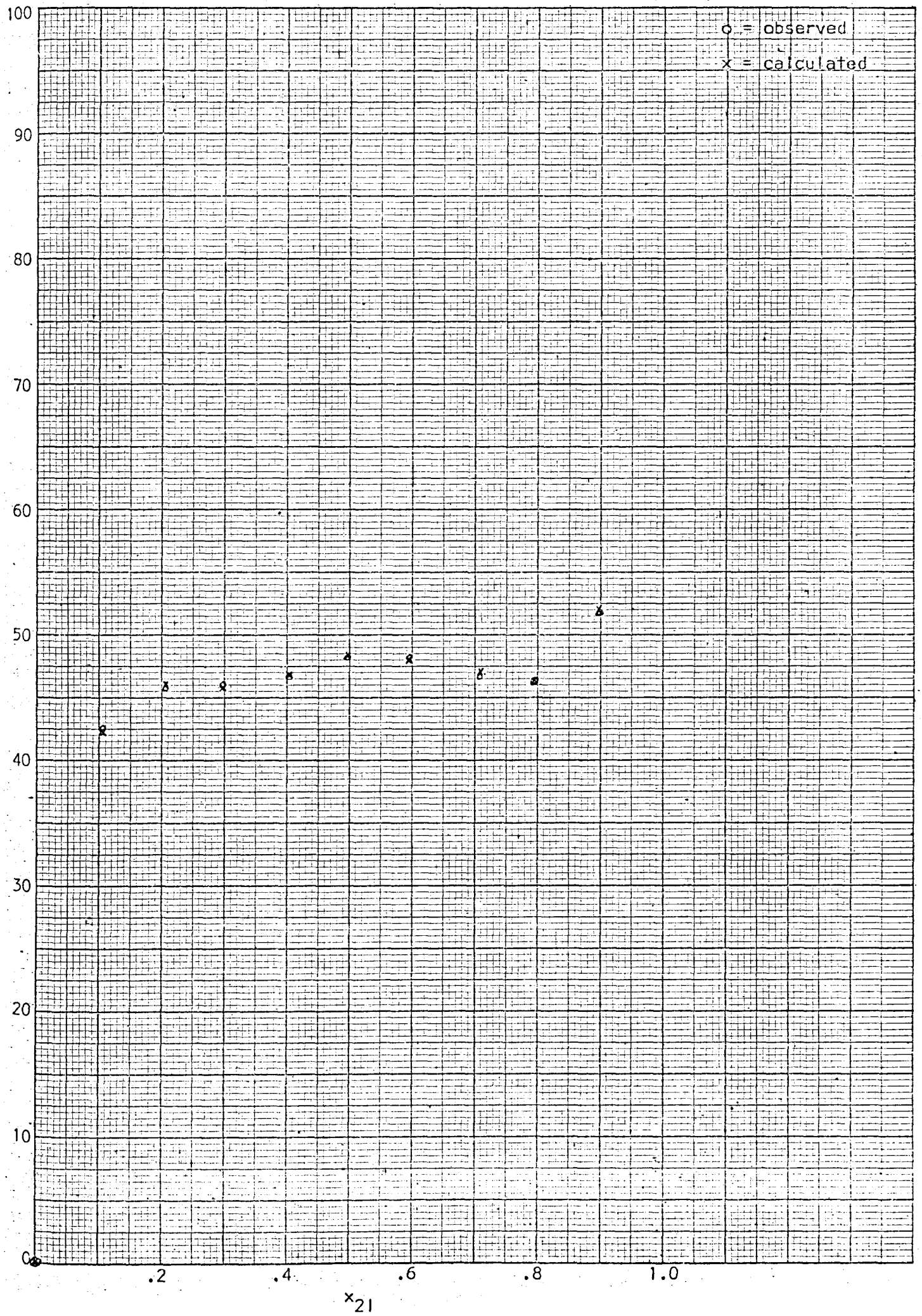
THERMODYNAMIC CONSISTENCY CURVE FITTING:

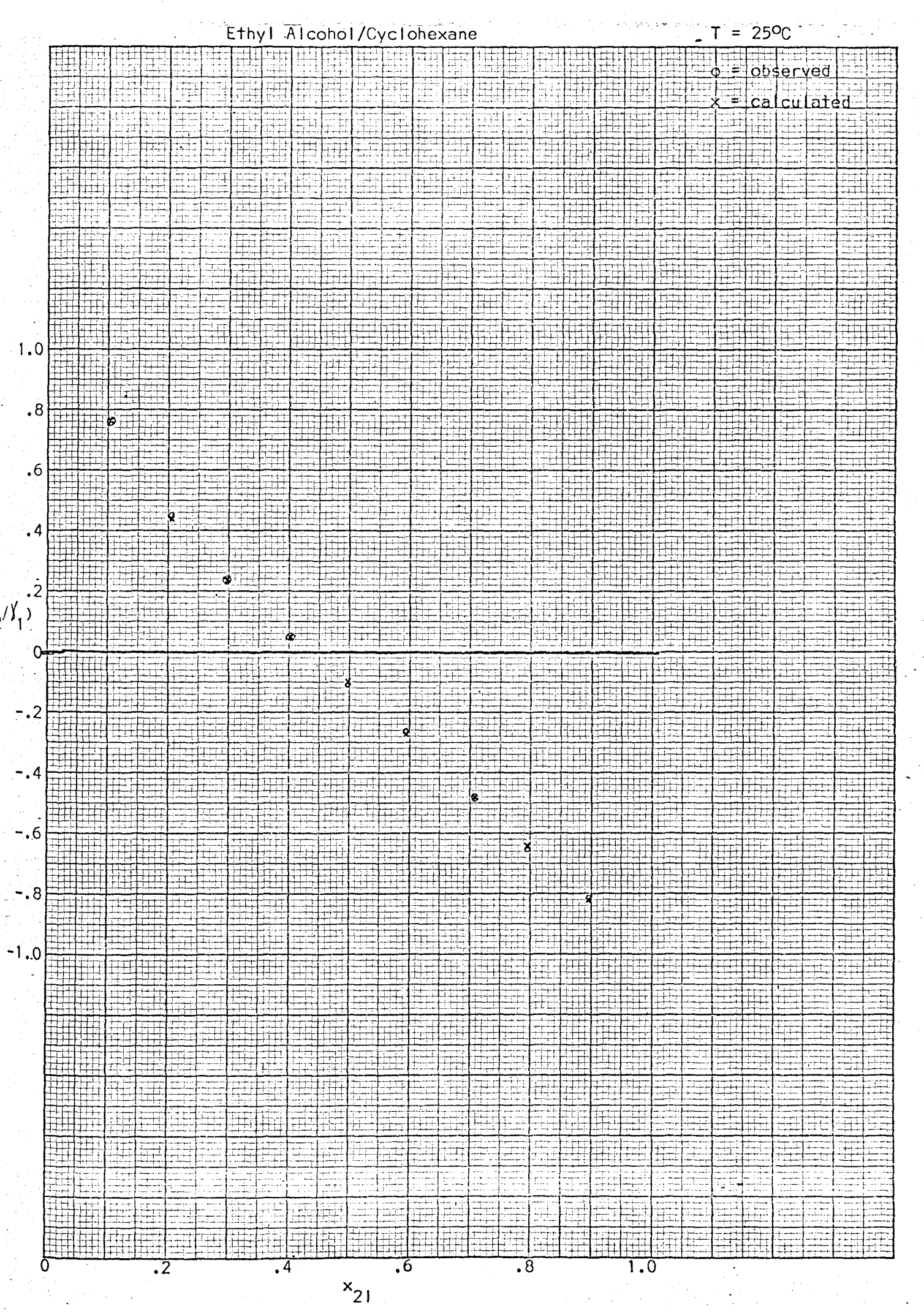
n	a_n	STD. ERROR	t	$\log(f_2/f_1)$ CALC.	DIF.
0	1.2622	0.0248	50.8863	-0.8158	0.0021
1	-5.9052	0.2991	-19.7456	-0.6415	-0.0064
2	12.0759	1.1216	10.7669	-0.4817	0.0026
3	-14.6068	1.6350	-8.9341	-0.2678	0.0075
4	6.2527	0.8101	7.7182	-0.1037	-0.0047
				0.0548	-0.0038
				0.2362	0.0015
				0.4443	0.0025
				0.7668	-0.0012

Degrees of Freedom= 4
Integral at x=1: -0.0663
Error in Integral: 0.0131

Ethyl Alcohol/Cyclohexane

T = 25°C




Ethyl Alcohol/Cyclohexane
T = 25°C
⊕ = observed
× = calculated
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
0
.2
.4
.6
.8
1.0
x_{21}

System: Ethyl Alcohol/Cyclohexane T=

Reference: Nagai J.,Isii N.:J. Soc. Chem, Ind. Japan 38,86(1935)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
116.90	0.9500	0.6330	73.9977	0.8199	5.2320	-0.8049
139.50	0.9000	0.5118	71.3961	0.8350	4.1527	-0.6966
153.50	0.8500	0.4515	69.3052	0.8583	3.4226	-0.6007
162.40	0.8000	0.4163	67.6071	0.8896	2.8900	-0.5117
167.90	0.7500	0.3949	66.3037	0.9306	2.4780	-0.4253
171.20	0.7000	0.3791	64.9019	0.9760	2.1605	-0.3451
174.00	0.6500	0.3673	63.9102	1.0350	1.9179	-0.2679
175.70	0.6000	0.3575	62.8127	1.1020	1.7208	-0.1936
177.00	0.5500	0.3486	61.7022	1.1809	1.5623	-0.1216
178.00	0.5000	0.3422	60.9116	1.2823	1.4279	-0.0467
178.60	0.4500	0.3382	60.4025	1.4129	1.3104	0.0327
178.90	0.4000	0.3349	59.9136	1.5767	1.2092	0.1152
179.10	0.3500	0.3339	59.8015	1.7985	1.1191	0.2060
178.90	0.3000	0.3315	59.3053	2.0809	1.0418	0.3005
178.60	0.2500	0.3298	58.9023	2.4801	0.9732	0.4063
178.00	0.2000	0.3275	58.2950	3.0682	0.9124	0.5267
176.90	0.1500	0.3223	57.0149	4.0010	0.8600	0.6677
175.00	0.1000	0.3149	55.1075	5.8008	0.8123	0.8538
169.70	0.0500	0.2923	49.6033	10.4428	0.7708	1.1319

PARTIAL PRESSURE CURVE FITTING:

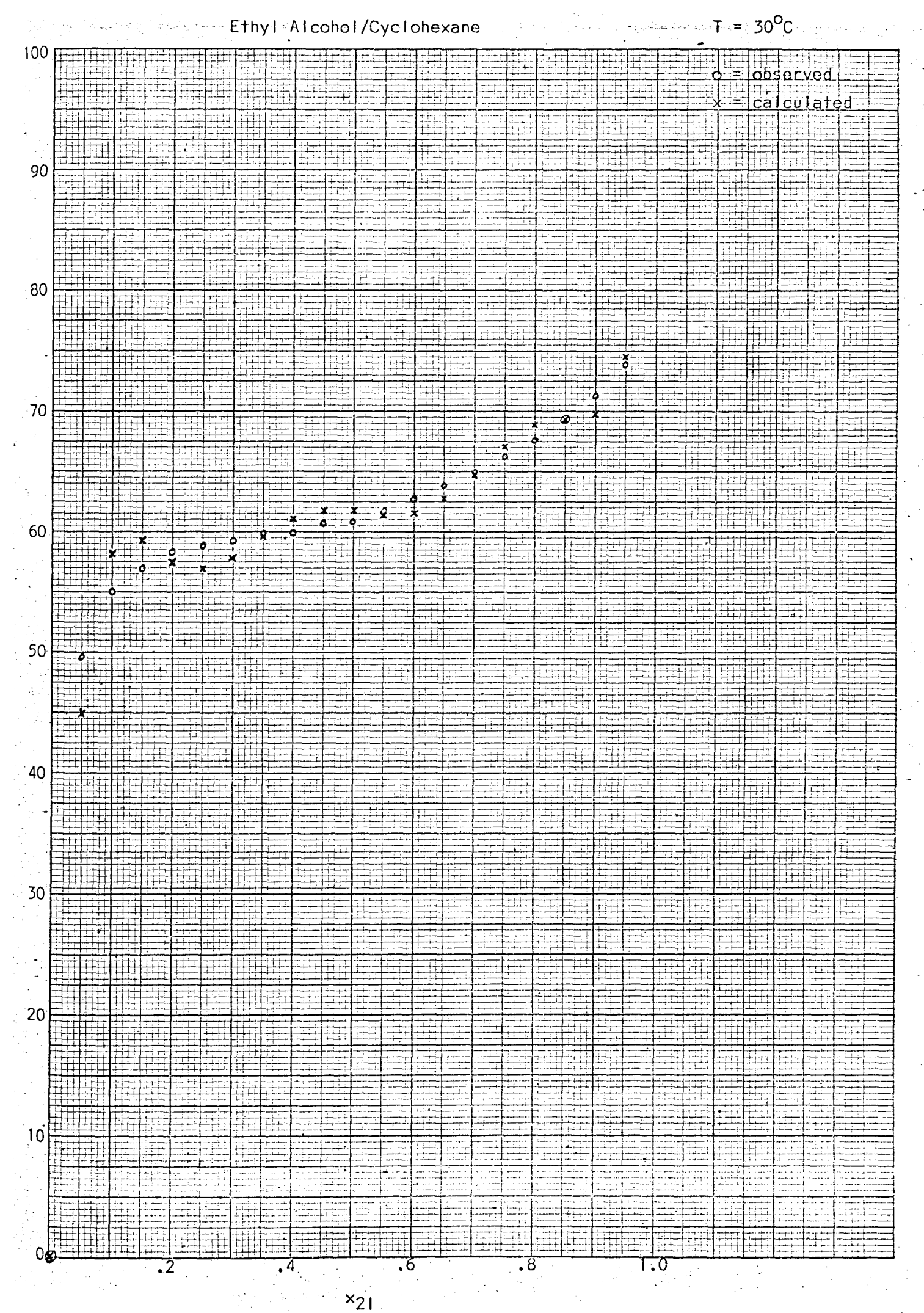
n	a_n	STD.ERROR	t
1	1409.9347	72.6784	19.3996
2	-12693.0345	1169.8739	-10.8499
3	55972.2879	7052.1233	7.9369
4	-133198.0922	20635.7766	-6.4547
5	176576.2680	31438.8828	5.5529
6	-118462.5470	23972.3872	-4.9416
7	32490.2698	7223.9489	4.4976

Degrees of Freedom= 13
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

P_2 CALC.	DIF.
74.6340	-0.6363
69.7943	1.6018
69.4332	-0.1279
68.8875	-1.2804
67.1252	-0.8215
64.7468	0.1551
62.7020	1.2082
61.5915	1.2213
61.4275	0.2747
61.7253	-0.8137
61.7957	-1.3932
61.1141	-1.2005
59.6341	0.1674
57.9213	1.3841
56.9771	1.9251
57.6256	0.6694
59.3349	-2.3200
58.3462	-3.2387
44.9809	4.6224

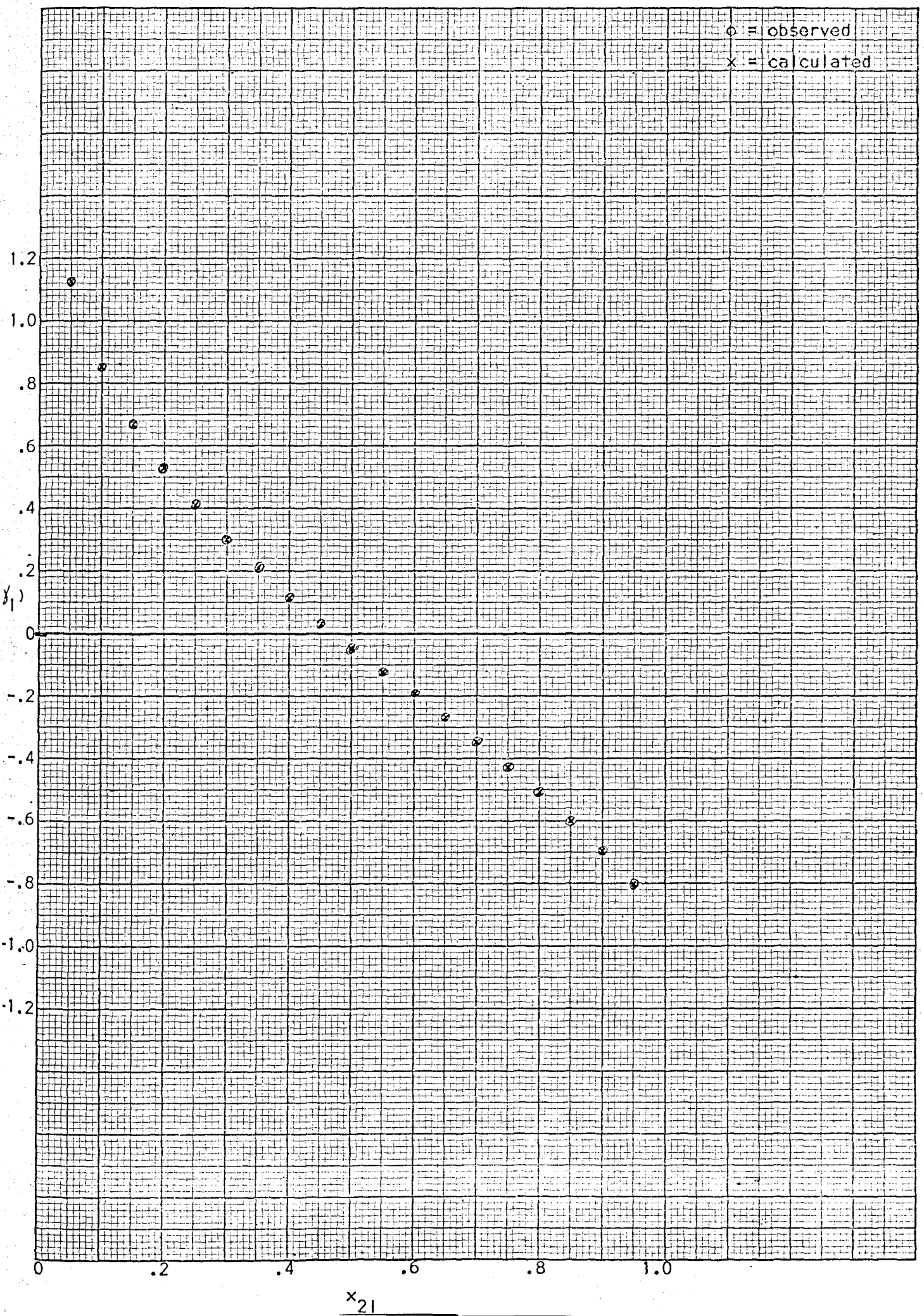
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.5651	0.0544	288.2053	-0.8049	0.0000
1	-10.9176	0.1602	-68.1515	-0.6966	-0.0001
2	52.5548	1.6197	32.4477	-0.6008	0.0001
3	-176.2019	7.7301	-22.7941	-0.5113	-0.0005
4	354.1195	19.5717	18.0935	-0.4260	0.0007
5	-411.8812	26.9996	-15.2551	-0.3450	-0.0002
6	254.5767	19.1479	13.2953	-0.2679	0.0000
7	-64.7577	5.4599	-11.8606	-0.1938	0.0002
				-0.1208	-0.0008
Degrees of Freedom= 11				-0.0464	-0.0003
Integral at x=1: 0.0253				0.0317	0.0010
Error in Integral: 0.0008				0.1152	0.0001
				0.2051	0.0009
				0.3021	-0.0016
				0.4073	-0.0010
				0.5252	0.0015
				0.6669	0.0008
				0.8551	-0.0013
				1.1315	0.0004


Ethyl Alcohol/Cyclohexane
T = 30°C
o = observed
x = calculated
100
90
80
70
60
50
40
30
20
10
0
.2
.4
.6
.8
1.0
x21

Ethyl Alcohol/Cyclohexane

T = 30°C



System: Butyl Alcohol/Benzene T= 25°C.

Reference: Allan B.B.,Lingo S.P.,Felsing W.A.:J. Phys. Chem. 43,425(1939)

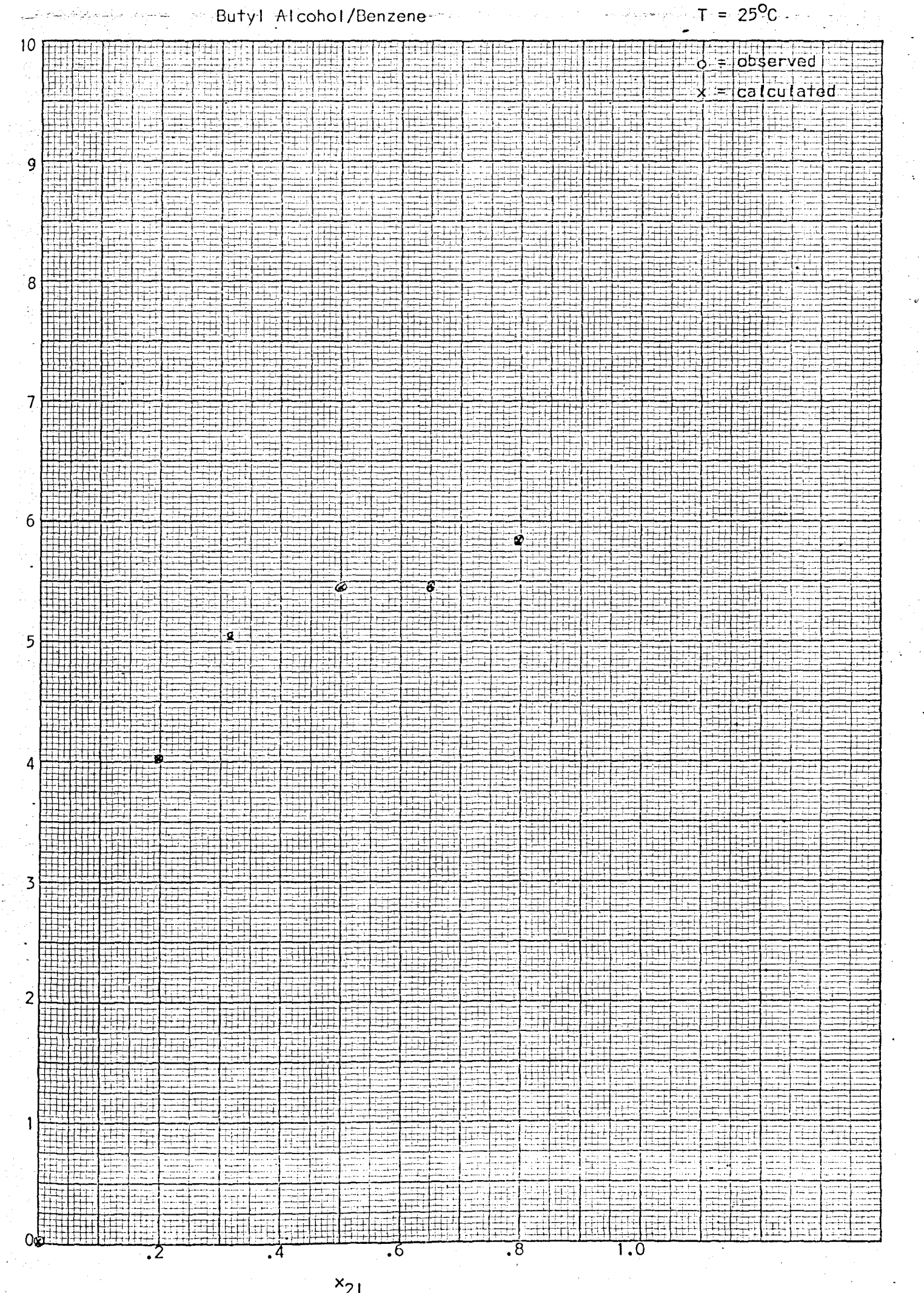
P_{12}	x_{2l}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
51.60	0.7980	0.1130	5.8308	0.2810	2.4104	-0.9333
67.40	0.6500	0.0810	5.4594	0.3230	1.8827	-0.7655
77.90	0.5000	0.0700	5.4530	0.4195	1.5414	-0.5652
85.80	0.3130	0.0590	5.0622	0.6220	1.2502	-0.3032
89.30	0.1970	0.0450	4.0185	0.7846	1.1298	-0.1584

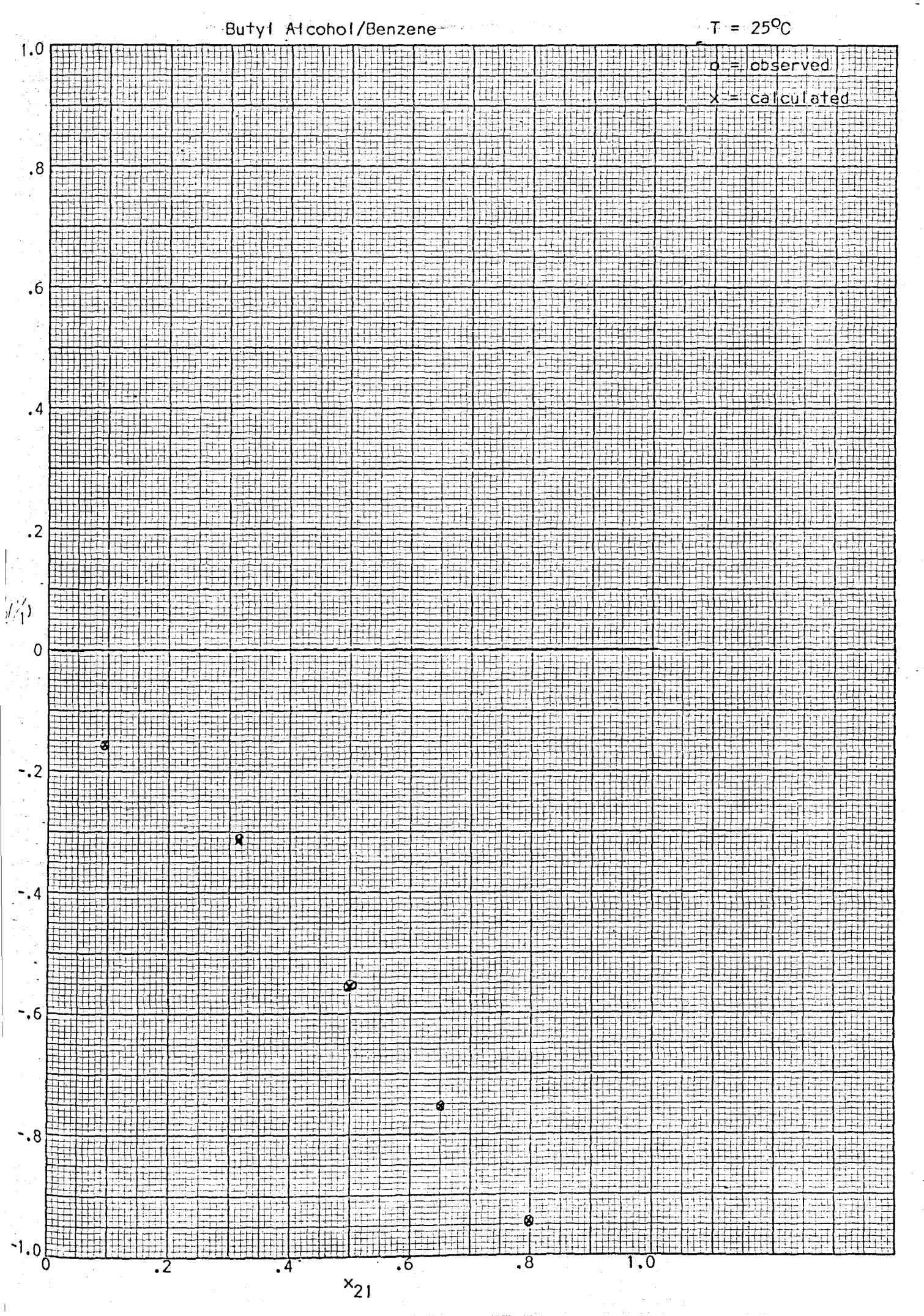
PARTIAL PRESSURE CURVE FITTING:

n	a_n	ST.ERROR	t	P_2 CALC.	DIF.
1	29.8262	0.1278	233.2960	5.8313	-0.0005
2	-53.8629	0.4690	-114.8478	5.4551	0.0043
3	32.1351	0.4074	78.8842	5.4643	-0.0113
				5.0441	0.0181
Degrees of Freedom= 3				4.0311	-0.0126
Confidence in First Term= 99.5%+					
Confidence in Last Term= 99.5%+					

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.0983	0.0140	7.0011	-0.9462	0.0129
1	-1.3089	0.0261	-50.1105	-0.7525	-0.0131
				-0.5561	-0.0091
Degrees of Freedom= 3				-0.3114	0.0082
Integral at x=1: -0.5561				-0.1595	0.0011
Error in Integral: 0.0099					


Butyl Alcohol/Benzene
T = 25°C
o = observed
x = calculated
10
9
8
7
6
5
4
3
2
1
0
.2
.4
.6
.8
1.0
x_{21}


Butyl Alcohol/Benzene
T = 25°C
o = observed
x = calculated
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
0
.2
.4
.6
.8
1.0
x_{21}

System: Butyl Alcohol/Benzene T= 45°C.

Reference: Brown I.,Smith F.:Austr. J. Chem. 12,407(1959)

p_{12}	x_{2l}	x_{2v}	p_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
114.04	0.8206	0.1893	21.5878	0.4551	2.2945	-0.7025
148.84	0.7072	0.1311	19.5129	0.4774	1.9666	-0.6149
171.29	0.6003	0.1054	18.0540	0.5203	1.7069	-0.5159
187.62	0.4915	0.0815	16.6044	0.5845	1.4974	-0.4086
197.33	0.4004	0.0779	15.3720	0.6642	1.3511	-0.3084
205.68	0.3007	0.0684	14.0685	0.8094	1.2200	-0.1782
212.80	0.1986	0.0579	12.3211	1.0734	1.1138	-0.0161
218.90	0.0974	0.0432	9.4565	1.6797	1.0331	0.2111
221.29	0.0538	0.0323	7.1477	2.2986	1.0077	0.3581

PARTIAL PRESSURE CURVE FITTING:

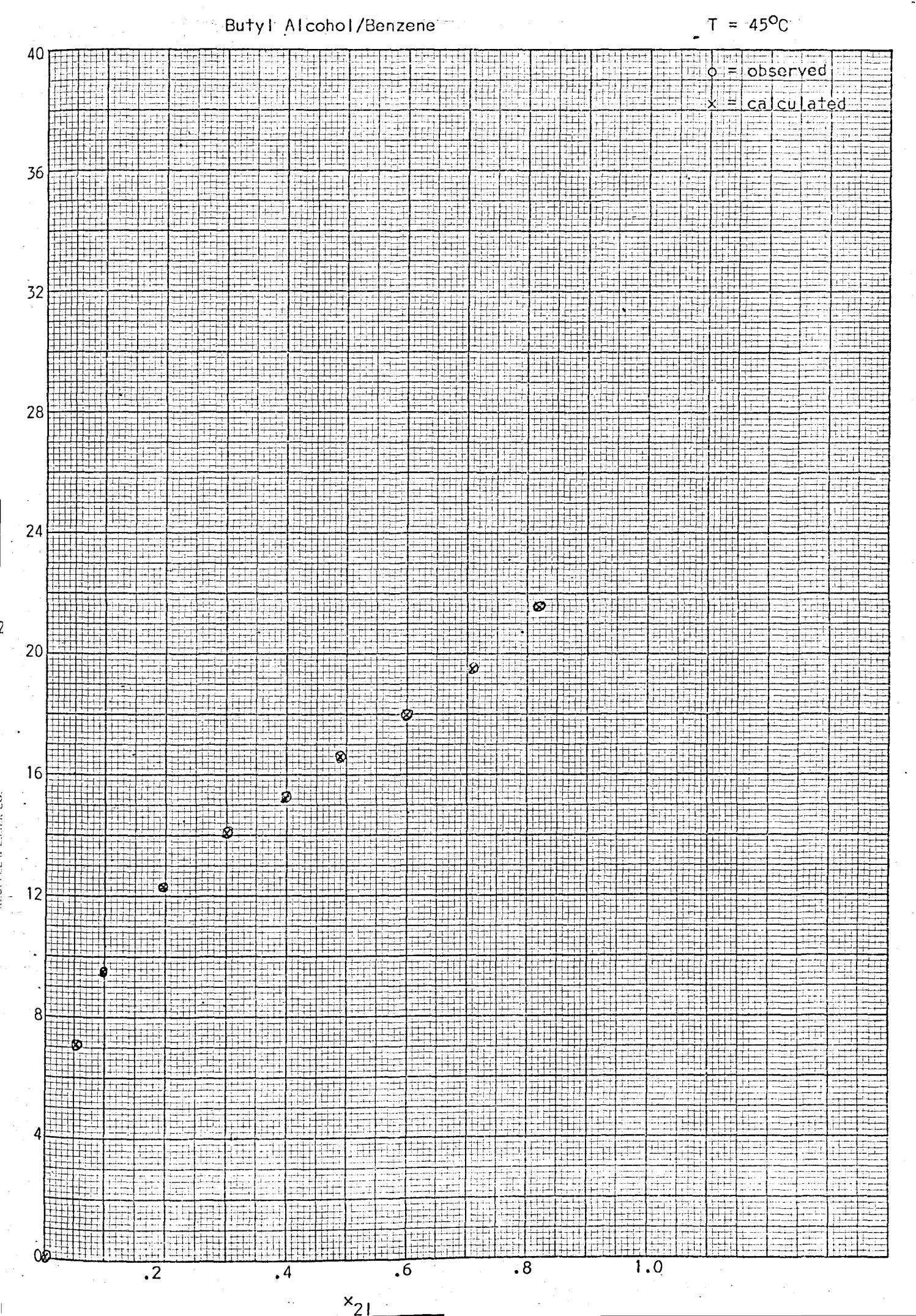
n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	214.9621	7.8860	27.2588	21.5874	0.0003
2	-2117.7799	216.1031	-9.7999	19.5141	-0.0012
3	13281.0898	2162.1289	6.1426	18.0482	0.0058
4	-50154.0113	10683.7246	-4.6944	16.6219	-0.0175
5	113797.3927	28900.2123	3.9376	15.3426	0.0294
6	-151140.5908	43532.9951	-3.4719	14.1000	-0.0315
7	107956.8301	34222.7289	3.1545	12.2950	0.0262
8	-31951.1923	10930.3195	-2.9232	9.4817	-0.0252
				7.1309	0.0168

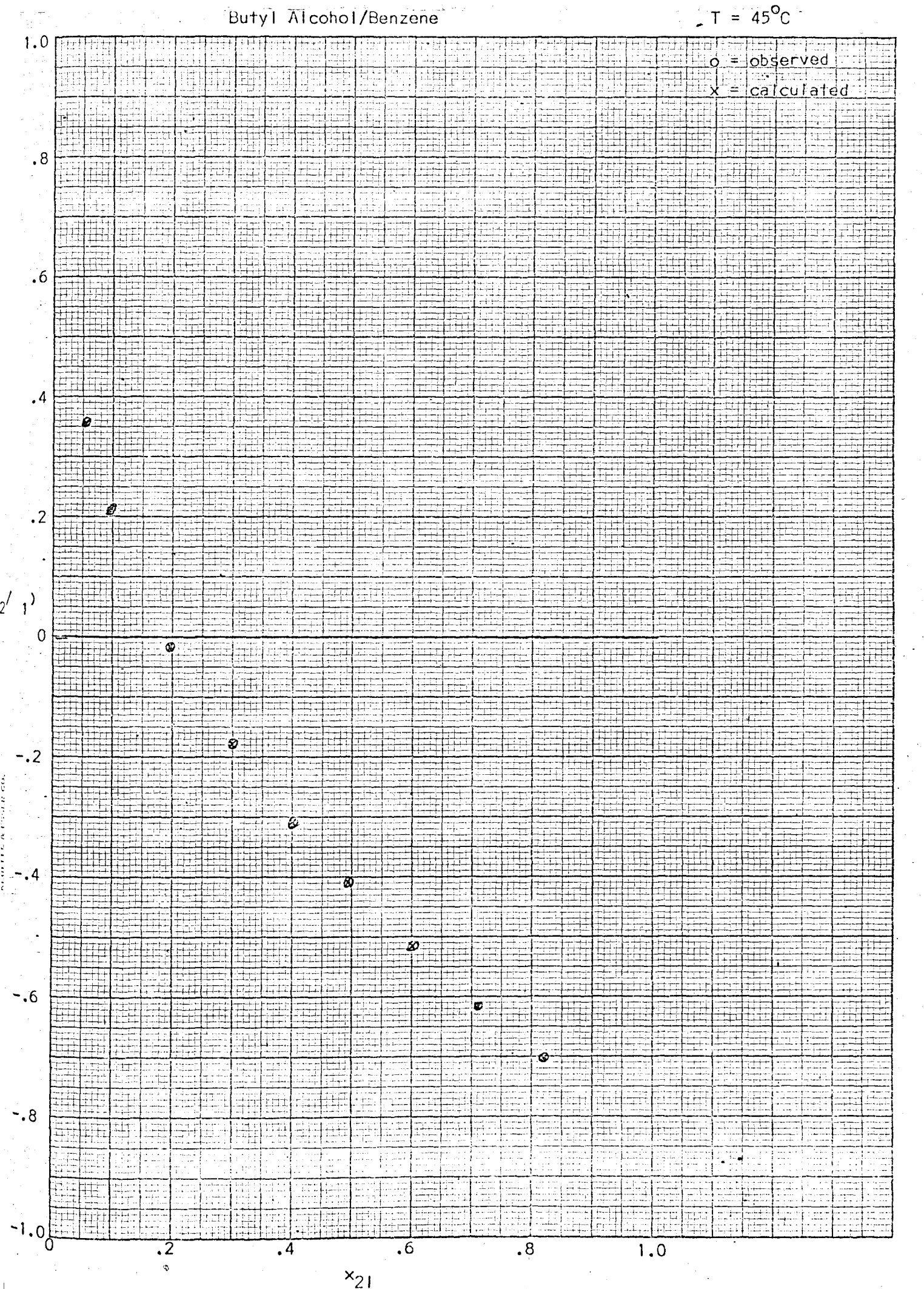
Degrees of Freedom= 2
Confidence in First Term= 99.5%+
Confidence in Last Term= 95.0%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.6149	0.0055	111.2044	-0.7025	0.0000
1	-5.8211	0.1514	-38.4546	-0.6151	0.0002
2	22.6445	1.3730	16.4929	-0.5154	-0.0006
3	-65.3600	5.6749	-11.5174	-0.4094	0.0008
4	110.1691	11.7220	9.3985	-0.3080	-0.0004
5	-97.2817	11.7618	-8.2710	-0.1779	-0.0002
6	34.6168	4.5574	7.5958	-0.0165	0.0005
				0.2115	-0.0004
				0.3580	0.0002

Degrees of Freedom= 2
Integral at x=1: -0.3220
Error in Integral: 0.0004


Butyl Alcohol/Benzene
T = 45°C
o = observed
x = calculated
40
36
32
28
24
20
16
12
8
4
0
.2
.4
.6
.8
1.0
x_{21}


Butyl Alcohol/Benzene
T = 45°C
o = observed
x = calculated
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
0
.2
.4
.6
.8
1.0
x_{21}

System: Ethyl Ether/Benzene T=. 20°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	f_2	γ_1	$\log(\gamma_2/\gamma_1)$
185.40	1.0000	1.0000	185.4000	1.0000	1.0000	0.0000
180.50	0.9563	0.9957	179.7238	1.0137	4.8527	-0.6801
176.40	0.8069	0.9908	174.7771	1.1683	2.2963	-0.2935
167.80	0.7591	0.9858	165.4172	1.1754	2.7025	-0.3616
157.90	0.5009	0.9839	155.3578	1.6729	1.3917	0.0799
133.20	0.2640	0.9774	130.1897	2.6599	1.1175	0.3766
84.50	0.0960	0.9585	80.9932	4.5506	1.0599	0.6328
42.80	0.0412	0.9149	39.1577	5.1264	1.0379	0.6936
3.66	0.0000	0.0000	0.0000	1.0000	1.0000	0.0000

PARTIAL PRESSURE CURVE FITTING:

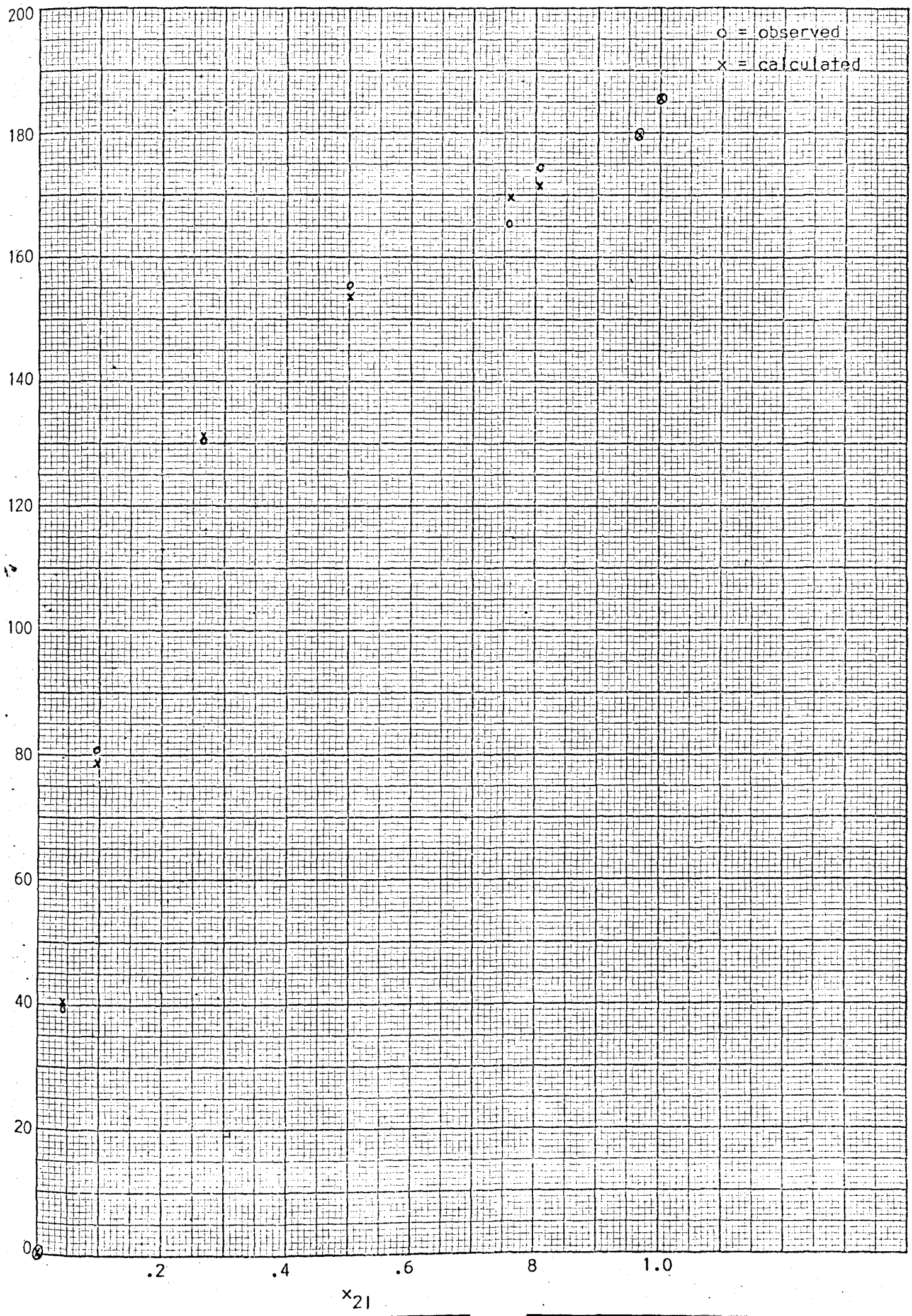
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	1126.7319	61.9566	18.1858	185.6123	-0.2123
2	-3759.4011	548.5219	-6.8537	179.6926	0.0313
3	6615.9086	1633.4307	4.0503	171.3525	3.4246
4	-5703.2137	1952.7782	-2.9206	169.5245	-4.1073
5	1905.5865	807.8945	2.3587	153.6688	1.6890
				131.9132	-1.7235
Degrees of Freedom= 4				78.9041	2.0892
Confidence in First Term= 99.5%+				40.4865	-1.3288
Confidence in Last Term= 95.0%+				0.0000	0.0000

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.7701	0.0398	19.3306	------	------
1	-1.4433	0.0670	-21.5367	-0.6102	-0.0699
				-0.3946	0.1011
Degrees of Freedom= 5				-0.3256	-0.0360
Integral at x=1: 0.0484				0.0471	0.0328
Error in Integral: 0.0506				0.3890	-0.0124
				0.6315	0.0013
				0.7106	-0.0169
				------	------

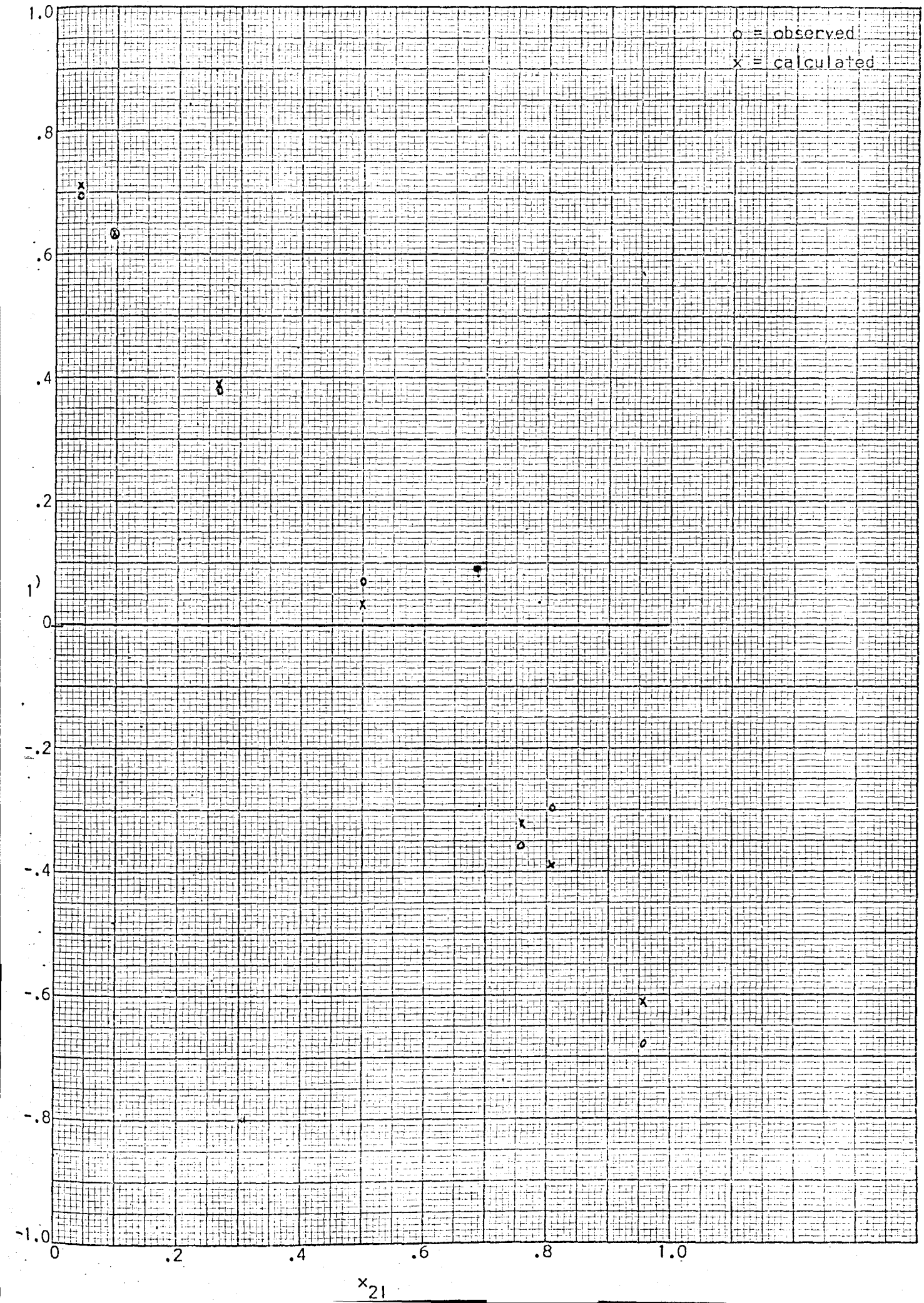
Ethyl Ether/Benzene

T = 20°C



Ethyl Ether/Benzene

T = 20°C



System: Ethyl Ether/Benzene T= 35°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

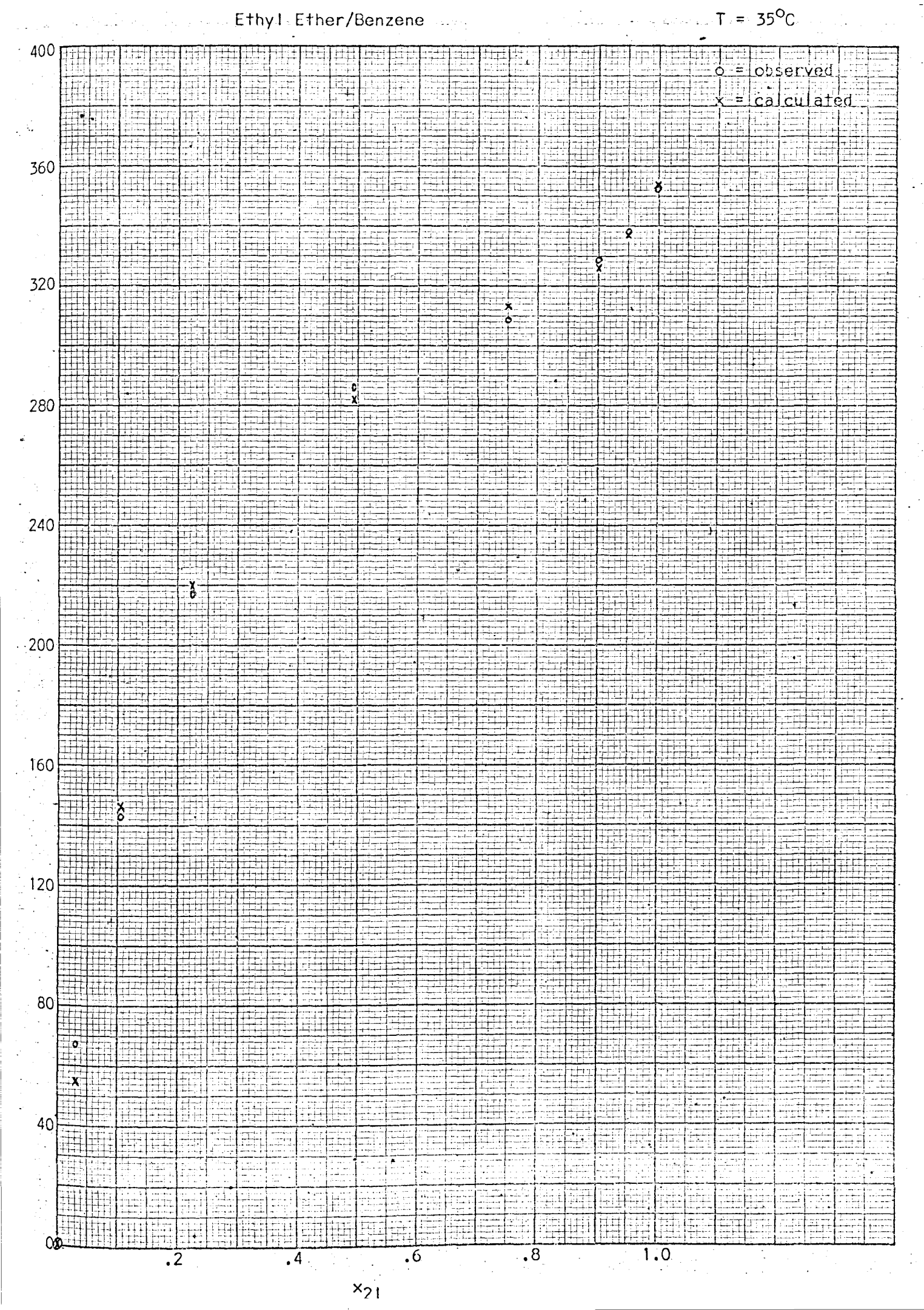
P_{12}	x_{2l}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
352.30	1.0000	1.0000	352.3000	1.0000	1.0000	------
340.40	0.9535	0.9935	338.1874	1.0068	5.4693	-0.7350
332.80	0.9008	0.9895	329.3056	1.0377	4.0489	-0.5913
314.20	0.7488	0.9832	308.9214	1.1710	2.4153	-0.3144
291.90	0.4942	0.9799	286.0328	1.6429	1.3333	0.0907
224.60	0.2249	0.9667	217.1208	2.7403	1.1091	0.3928
151.40	0.1053	0.9451	143.0881	3.8571	1.0678	0.5578
75.80	0.0316	0.8888	67.3710	6.0516	1.0005	0.7817
8.70	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	1949.2114	144.3890	13.4997	354.1089	-1.8089
2	-6486.7633	1290.1112	-5.0281	337.0553	1.1321
3	11909.1813	3742.8263	3.1819	326.1356	3.1700
4	-10852.1880	4337.3684	-2.5020	313.4912	-4.5697
5	3834.6674	1746.5029	2.1956	282.1644	3.8684
				220.1921	-3.0713
Degrees of Freedom= 4				145.9464	-2.8583
Confidence in First Term= 99.5%+				55.4827	11.8883
Confidence in Last Term= 95.0%+				0.0000	0.0000

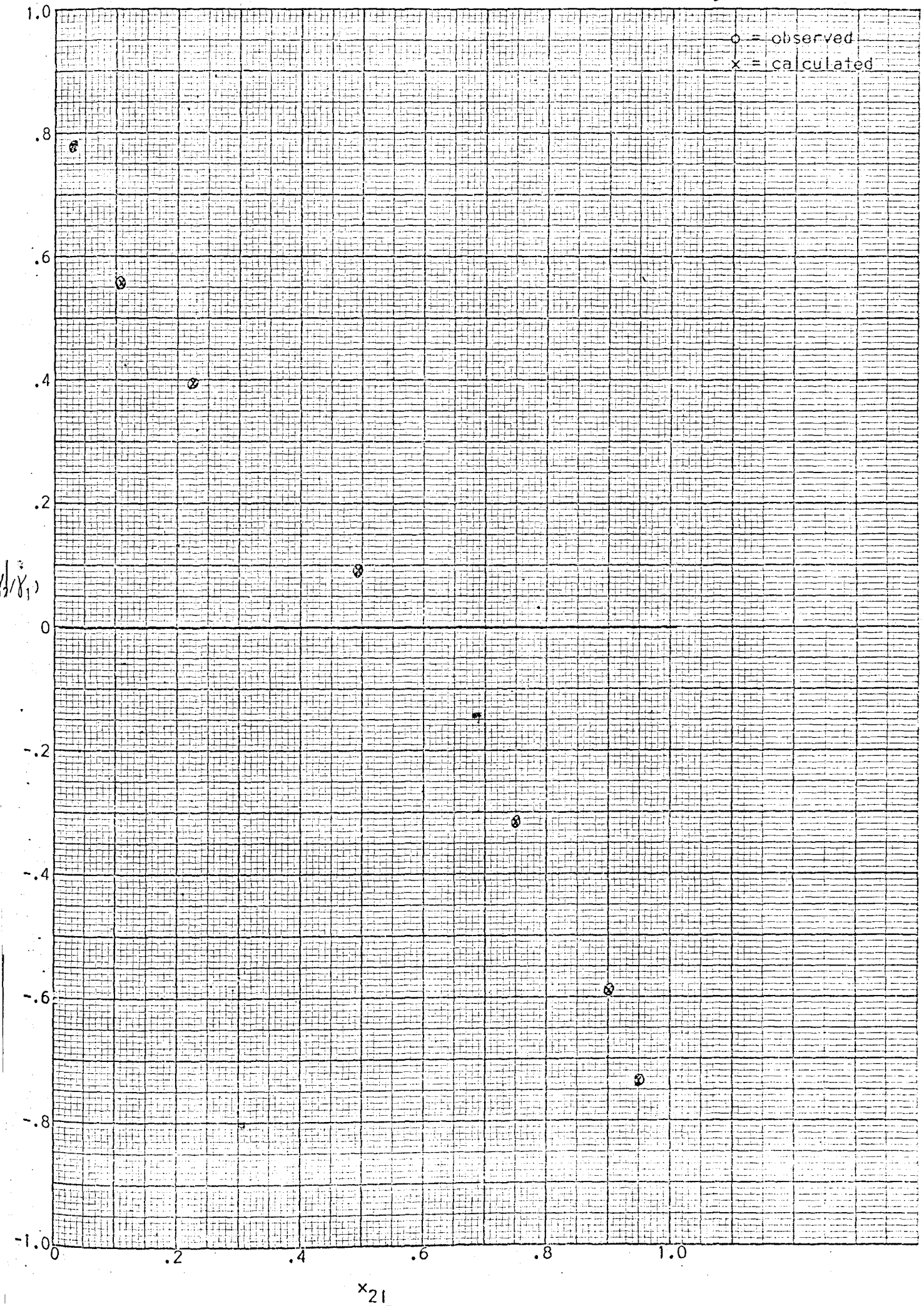
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.9313	0.0011	827.8218	------	------
1	-5.3958	0.0288	-187.1749	-0.7351	0.0001
2	22.3646	0.2058	108.6897	-0.5910	-0.0003
3	-50.5862	0.5635	-89.7655	-0.3146	0.0002
4	50.8096	0.6482	78.3839	0.0908	-0.0002
5	-19.0322	0.2644	-71.9846	0.3926	0.0002
				0.5580	-0.0003
Degrees of Freedom= 1				0.7816	0.0001
Integral at x=1: 0.0316				------	------
Error in Integral: 0.0002					


Ethyl Ether/Benzene
T = 35°C
o = observed
x = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x21

Ethyl Ether/Benzene

T = 35°C



System: Isopropyl Alcohol/Benzene. T= 25°C.

Reference: Olsen, Washburn(1937):Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	f_2	γ_1	$\log(\gamma_2/\gamma_1)$
104.50	0.0590	0.1260	13.1670	5.2265	0.9706	0.7312
109.00	0.1460	0.2050	22.3450	3.5843	1.0147	0.5481
108.40	0.3620	0.2550	27.6420	1.7883	1.2658	0.1501
105.80	0.5210	0.2880	30.4704	1.3697	1.5726	-0.0600
99.80	0.7000	0.3650	36.4270	1.2187	2.1124	-0.2389
84.10	0.8360	0.4700	39.5270	1.1073	2.7179	-0.3900
66.40	0.9200	0.6350	42.1640	1.0733	3.0295	-0.4506

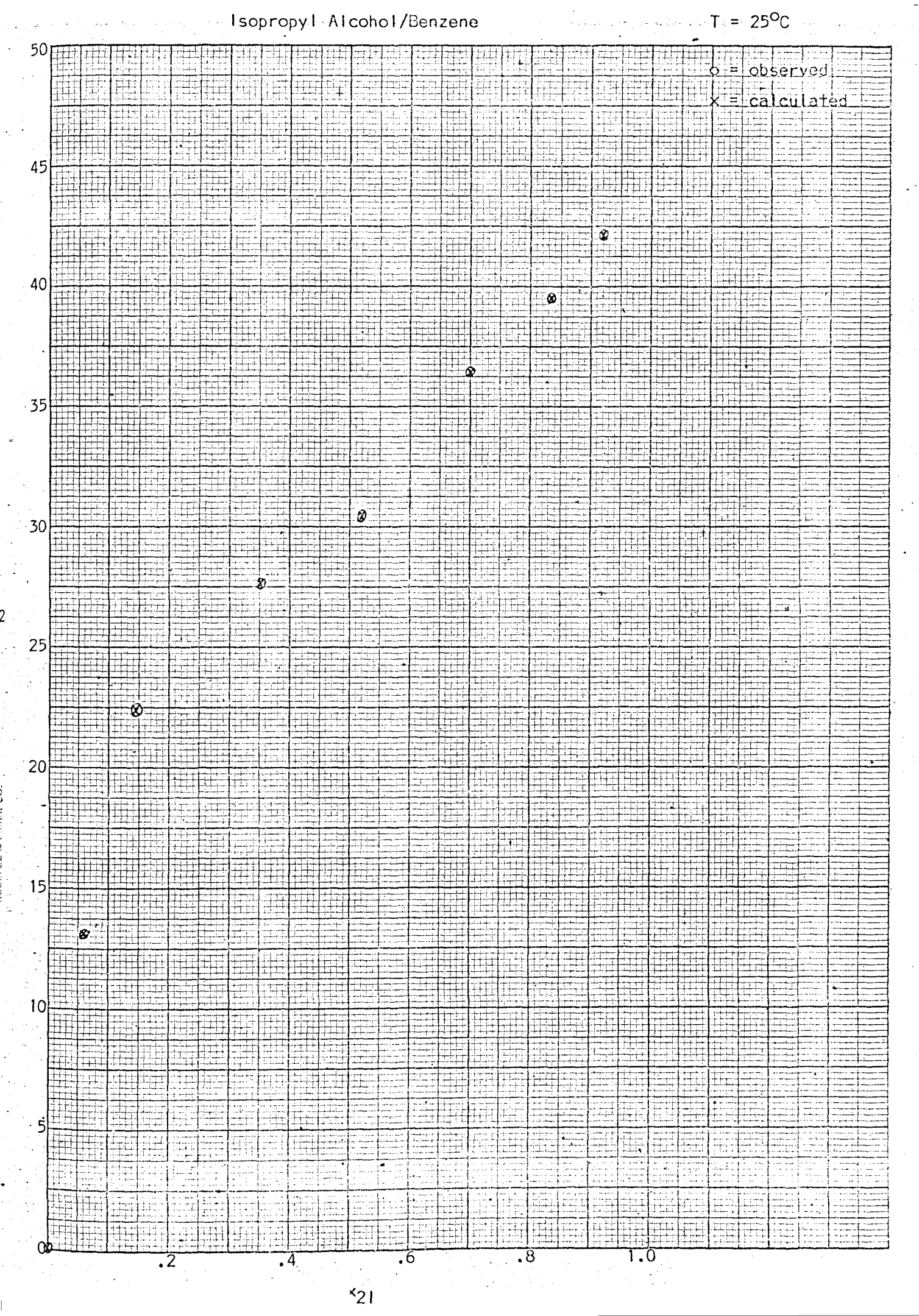
PARTIAL PRESSURE CURVE FITTING:

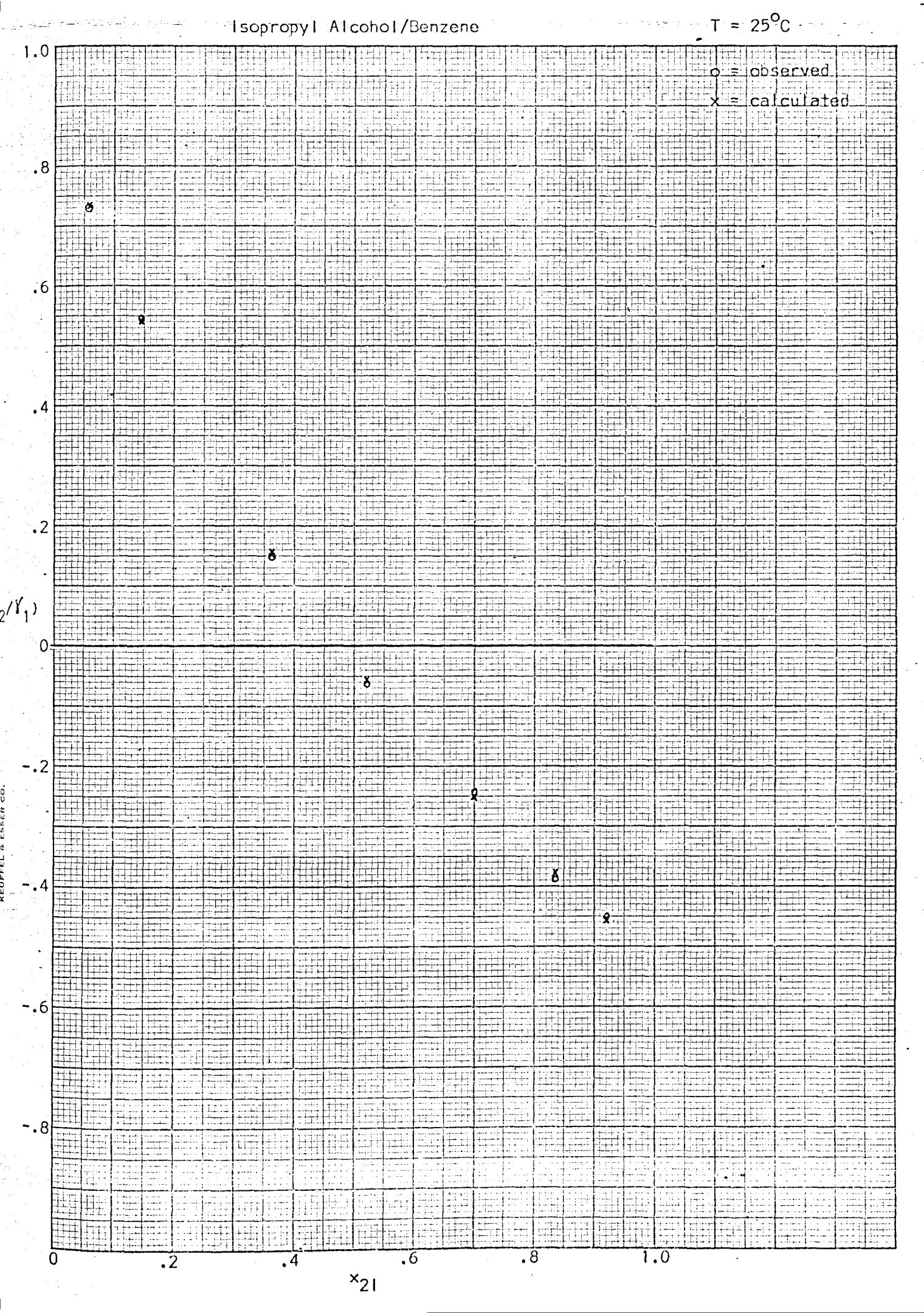
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	296.5733	1.0334	286.9799	13.1670	0.0000
2	-1481.3656	18.1972	-81.4063	22.3450	0.0000
3	4524.0960	114.6601	39.4566	27.6420	0.0000
4	-9228.3089	347.3940	-26.5644	30.4704	0.0000
5	12406.1895	546.6950	22.6931	36.4270	0.0000
6	-9465.7428	429.9724	-22.0148	39.5270	0.0000
7	3001.3463	133.4649	22.4879	42.1640	0.0000

Degrees of Freedom= 1
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.8828	0.0179	49.4147	0.7353	-0.0041
1	-2.6126	0.1826	-14.3111	0.5403	0.0078
2	1.9308	0.4440	4.3491	0.1555	-0.0054
3	-0.7301	0.2981	-2.4488	-0.0575	-0.0025
				-0.2503	0.0114
Degrees of Freedom= 3				-0.3784	-0.0115
Integral at x=1: 0.0376				-0.4550	0.0044
Error in Integral: 0.0075					


Isopropyl Alcohol/Benzene
T = 25°C
o = observed
x = calculated
50
45
40
35
30
25
20
15
10
5
0
.2
.4
.6
.8
1.0
x21


Isopropyl Alcohol/Benzene
T = 25°C
o = observed
x = calculated
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
γ_2/γ_1
0
.2
.4
.6
.8
1.0
x_{21}
KEUFFEL & ESSER CO.

System: Isopropyl Alcohol/Benzene T= 45°C.

Reference: Brown,Fock,and Smith(1956):Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
252.50	0.0472	0.1467	37.0417	5.7683	0.9344	0.79(
264.13	0.0980	0.2066	54.5693	4.0928	0.9600	0.62(
272.06	0.2047	0.2663	72.4496	2.6015	1.0371	0.39(
273.40	0.2960	0.2953	80.7350	2.0048	1.1309	0.24(
272.23	0.3862	0.3211	87.4098	1.6636	1.2442	0.12(
269.49	0.4763	0.3463	93.3244	1.4402	1.3900	0.01(
264.92	0.5504	0.3693	97.8350	1.3065	1.5357	-0.07(
259.35	0.6198	0.3951	102.4692	1.2152	1.7051	-0.14(
247.70	0.7096	0.4378	108.4431	1.1233	1.9815	-0.24(
227.14	0.8073	0.5107	116.0004	1.0562	2.3833	-0.35(
189.28	0.9120	0.6658	126.0226	1.0157	2.9704	-0.46(
159.80	0.9655	0.8252	131.8670	1.0039	3.3457	-0.52(
136.05	1.0000	1.0000	136.0500	1.0000	1.0000	-----

PARTIAL PRESSURE CURVE FITTING:

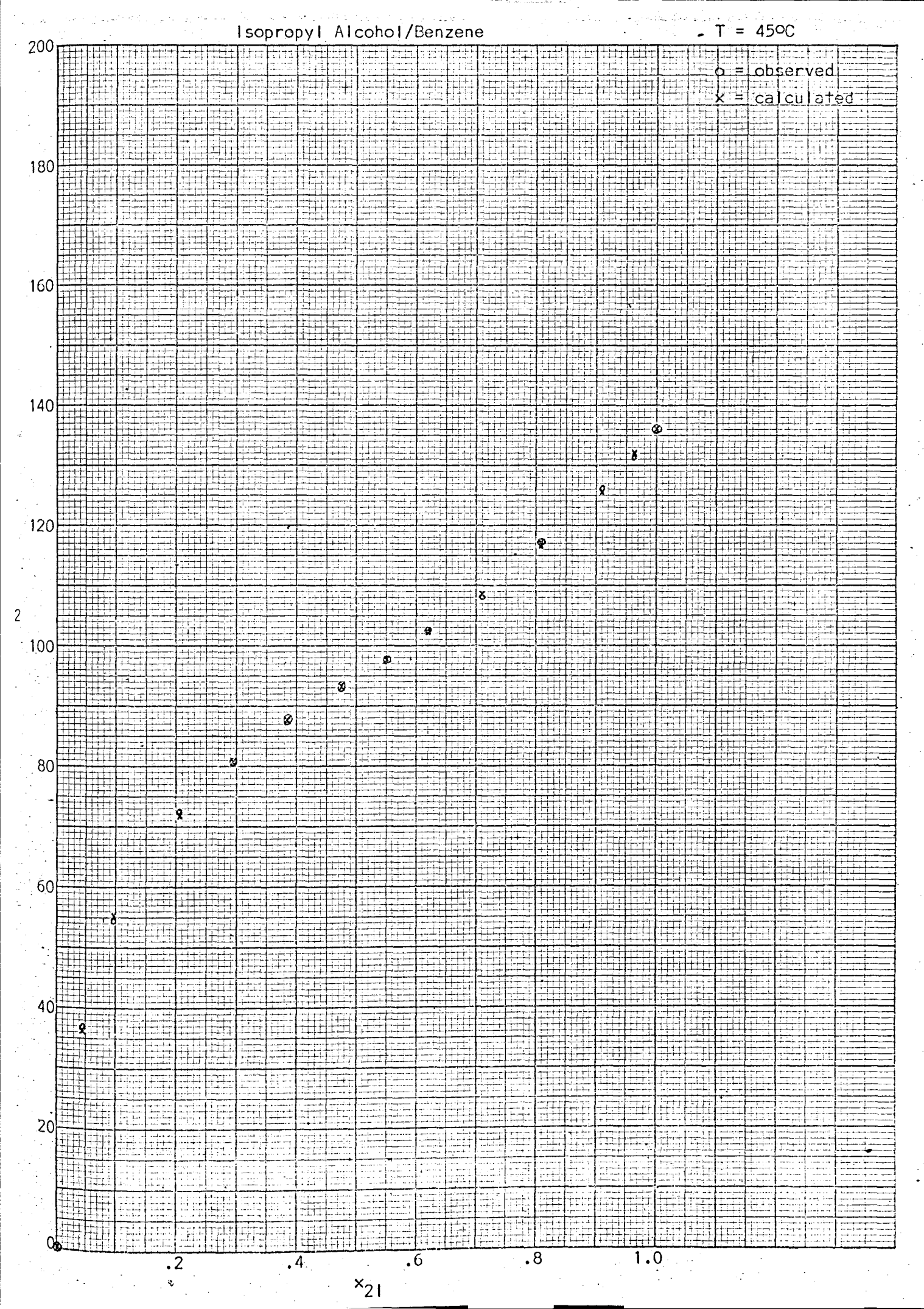
n	a_n	STD.ERROR	t
1	1075.9311	25.4674	42.2474
2	-7967.4457	542.4602	-14.6876
3	36454.1976	4228.1316	8.6218
4	-100621.2401	16219.1249	-6.2039
5	168616.2595	34032.3239	4.9546
6	-167305.2076	39815.0687	-4.2021
7	90244.0795	24371.0442	3.7029
8	-20360.6438	6080.5181	-3.3485

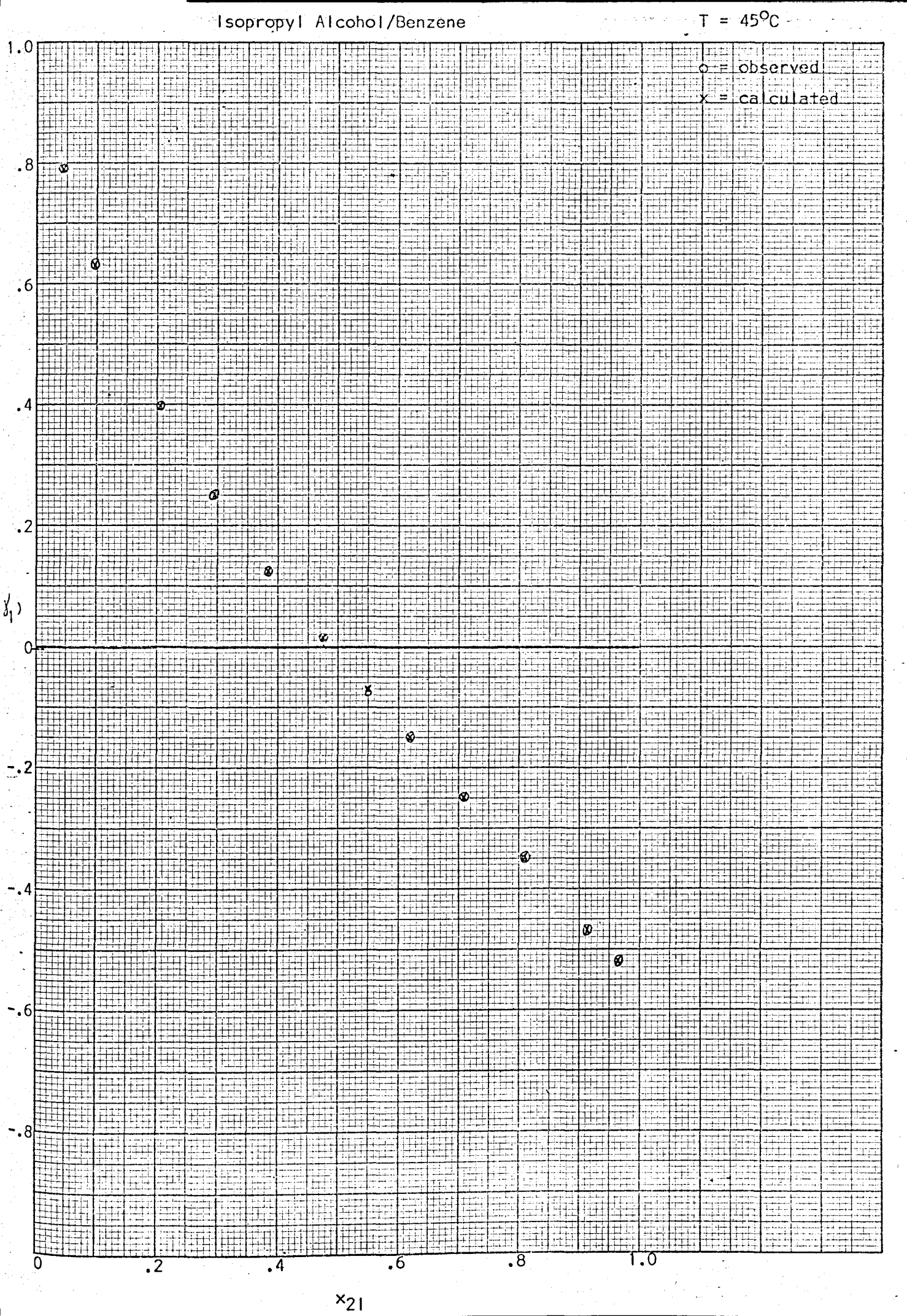
Degrees of Freedom= 6
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.0%+

P_2 CALC.	DIF.
36.4053	0.6364
55.3349	-0.7657
71.9916	0.4580
80.7692	-0.0341
87.6912	-0.2813
93.2655	0.0589
97.7272	0.1078
102.3089	0.1603
108.7100	-0.2670
115.9649	0.0355
125.7920	0.2306
132.1638	-0.2968
135.9305	0.1195

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.9929	0.0065	152.9148	0.7903	0.0002
1	-5.0340	0.1979	-25.4413	0.6304	-0.0007
2	18.0748	2.0135	8.9768	0.3980	0.0013
3	-54.6074	9.6039	-5.6859	0.2502	-0.0016
4	105.3963	24.1889	4.3572	0.1257	0.0005
5	-121.3930	33.0778	-3.6699	0.0148	0.0006
6	75.1781	23.1940	3.2413	-0.0699	-0.0002
7	-19.1703	6.5274	-2.9369	-0.1470	-0.0001
				-0.2462	-0.0003
Degrees of Freedom= 4				-0.3539	0.0005
Integral at x=1: 0.0395				-0.4657	-0.0003
Error in Integral: 0.0007				-0.5229	0.0001
				---	---


Isopropyl Alcohol/Benzene
T = 45°C
o = observed
x = calculated
200
180
160
140
120
100
80
60
40
20
0
.2
.4
.6
.8
1.0
x_{21}


Isopropyl Alcohol/Benzene
T = 45°C
o = observed
x = calculated
1.0
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
γ_1)
0
.2
.4
.6
.8
1.0
x_{21}

System: Fluorobenzene/Cyclohexane T= 49°C.

Reference: Bhattacharyya,Anantaramav,Palit:Transaction Farad.Soc. 59,110(1963)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
229.86	1.0000	1.0000	229.8600	1.0000	1.0000	------
245.13	0.9321	0.8846	216.8420	1.0121	1.5280	-0.1789
252.07	0.8607	0.7823	197.2019	0.9968	1.4447	-0.1611
266.09	0.7513	0.6614	175.9813	1.0190	1.3292	-0.1154
279.19	0.6600	0.5899	164.6970	1.0855	1.2356	-0.0562
284.69	0.5913	0.5071	144.3635	1.0621	1.2597	-0.0741
278.34	0.5332	0.4801	133.6366	1.0903	1.1374	-0.0184
286.27	0.4764	0.4403	126.0504	1.1510	1.1227	0.0108
294.60	0.3597	0.3513	103.5048	1.2517	1.0950	0.0581
291.26	0.2424	0.2666	77.6412	1.3935	1.0345	0.1294
286.12	0.1441	0.1681	48.0910	1.4522	1.0203	0.1533
272.57	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	382.0226	13.7306	27.8226
2	-332.3712	40.1242	-8.2836
3	181.6549	27.9592	6.4971

Degrees of Freedom= 9
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

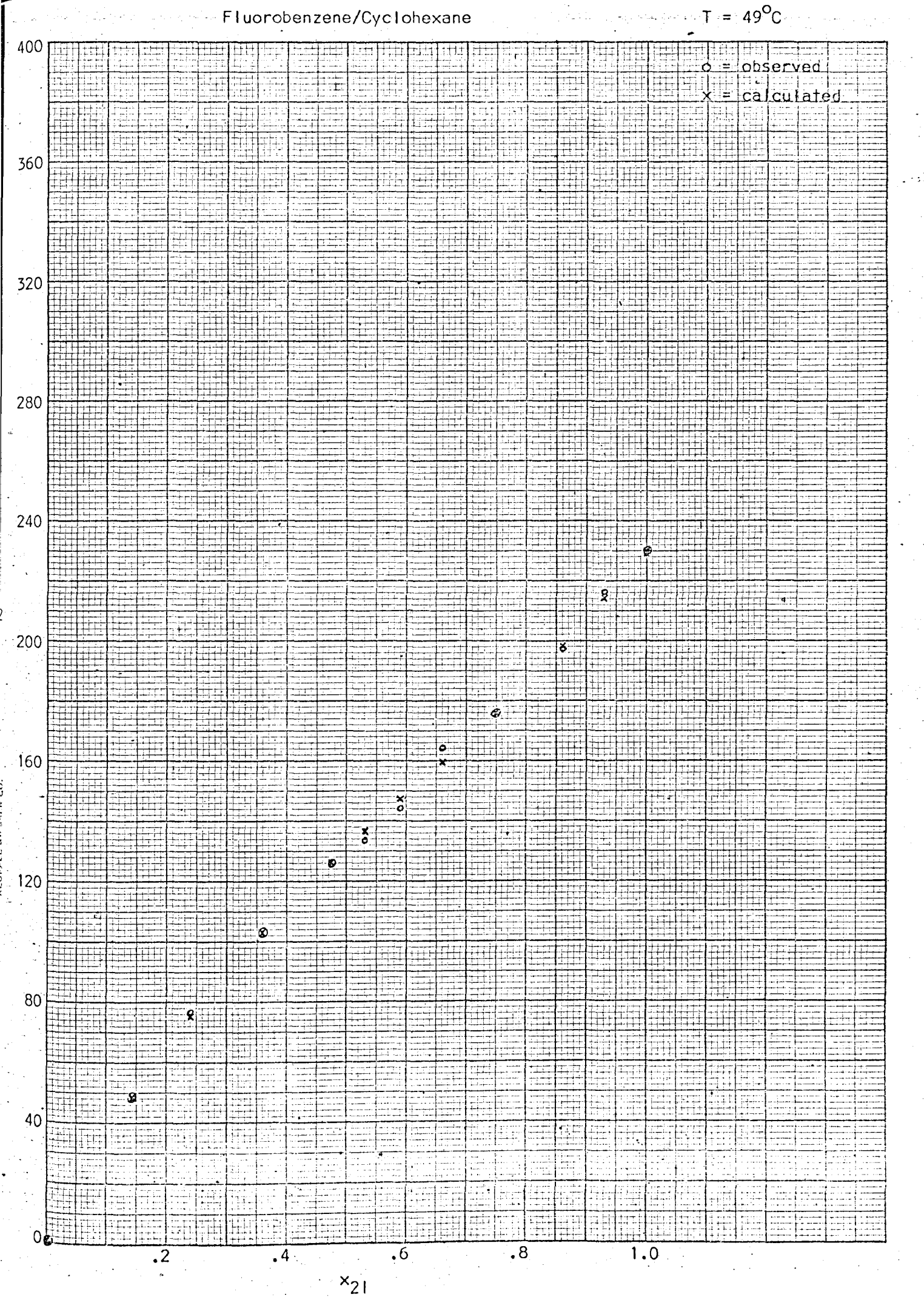
P_2 CALC.	DIF.
231.3064	-1.4464
214.4185	2.4235
198.4014	-1.1914
176.4391	-0.4578
159.5882	5.1088
147.2382	-2.8748
136.7431	-3.1065
126.2064	-0.1560
102.8727	0.6321
75.6602	1.9810
48.6825	-0.5914
0.0000	0.0000

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.2191	0.0117	18.6641
1	-0.4402	0.0194	-22.7447

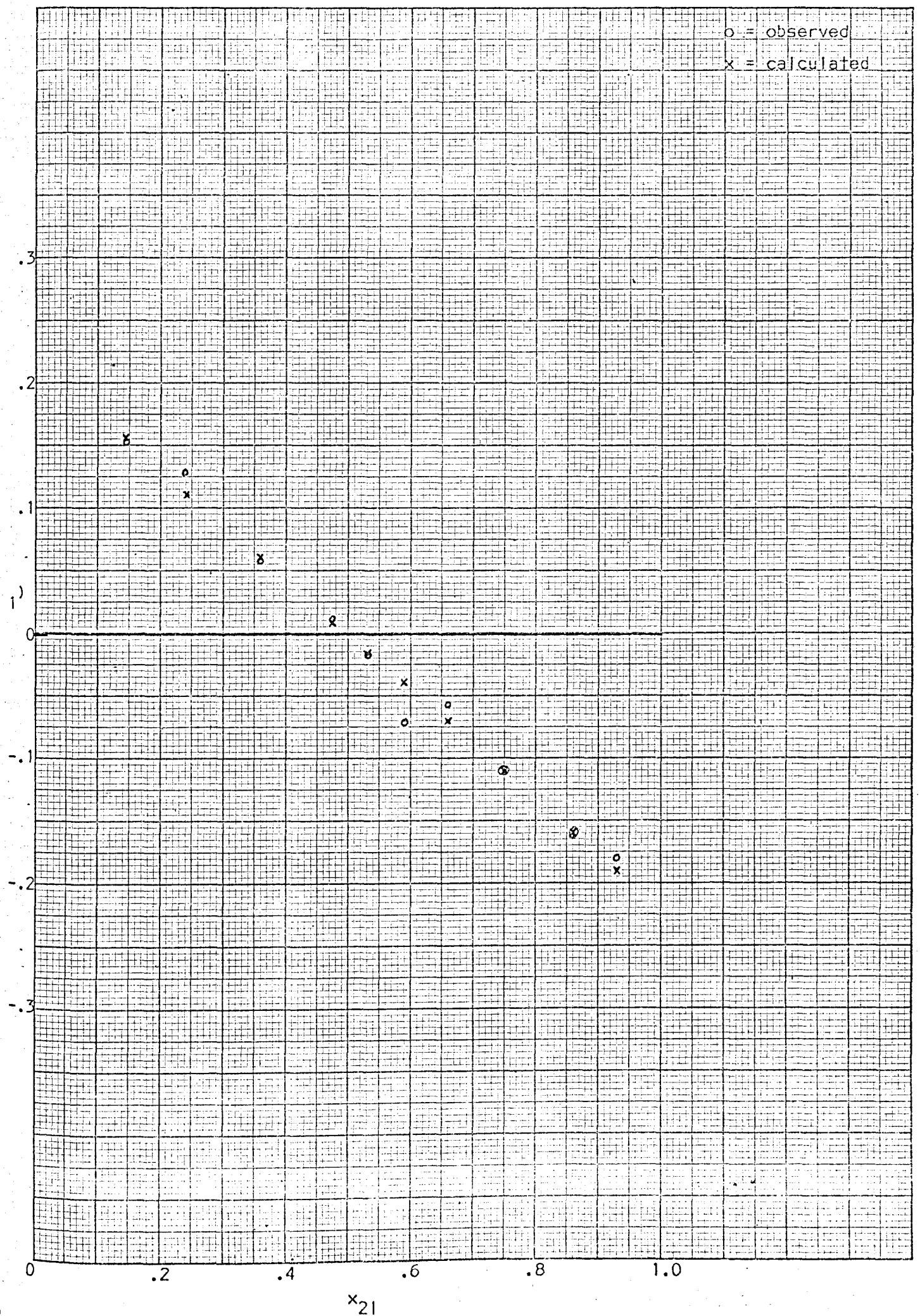
Degrees of Freedom= 8
Integral at x=1: -0.0010
Error in Integral: 0.0134

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
------	------
-0.1912	0.0123
-0.1597	-0.0014
-0.1116	-0.0038
-0.0714	0.0152
-0.0412	-0.0329
-0.0156	-0.0027
0.0094	0.0014
0.0608	-0.0027
0.1124	0.0170
0.1557	-0.0024
------	------


Fluorobenzene/Cyclohexane
T = 49°C
o = observed
x = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x_{21}

Fluorobenzene/Cyclohexane

T = 49°C



System: Fluorobenzene/Cyclohexane T= 59°C.

Reference: Bhattacharyya, Anantaramav, Palit: Transaction Farad.Soc. 59, 110(1963)

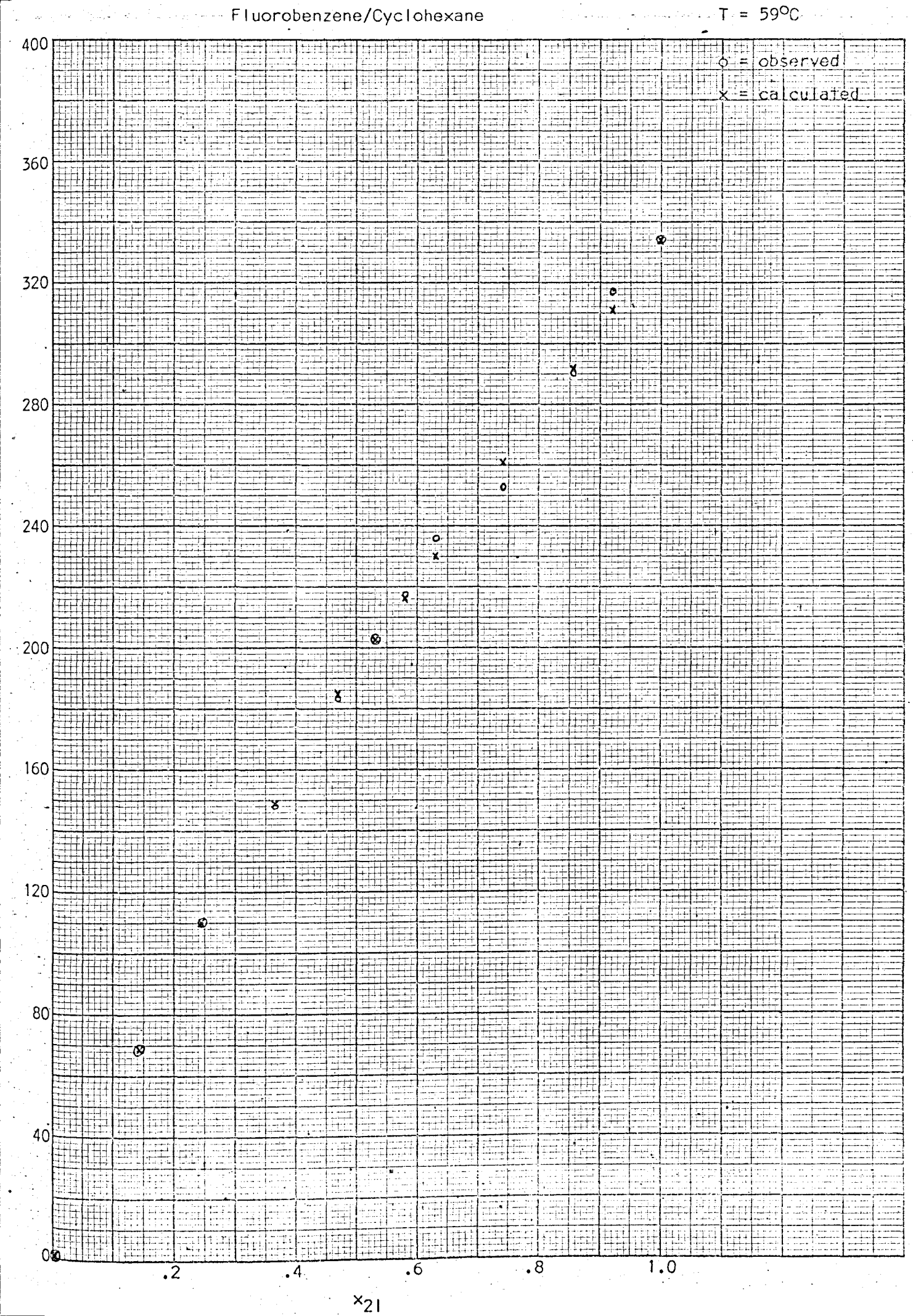
P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
333.90	1.0000	1.0000	333.9000	1.0000	1.0000	------
356.84	0.9217	0.8897	317.4663	1.0315	1.2913	-0.0975
366.98	0.8548	0.7907	290.1601	1.0166	1.3584	-0.1259
387.52	0.7429	0.6530	253.0351	1.0201	1.3428	-0.1194
402.92	0.6308	0.5879	236.8847	1.1247	1.1543	-0.0113
412.02	0.5796	0.5275	217.3529	1.1230	1.1887	-0.0247
416.18	0.5317	0.4884	203.2831	1.1451	1.1669	-0.0082
417.48	0.4693	0.4391	183.3363	1.1701	1.1324	0.0142
415.86	0.3564	0.3564	148.2167	1.2455	1.0675	0.0670
414.83	0.2461	0.2667	110.6393	1.3464	1.0357	0.1139
408.96	0.1437	0.1680	68.7175	1.4325	1.0199	0.1475
389.58	0.0000	0.0000	0.0000	1.0000	1.0000	------

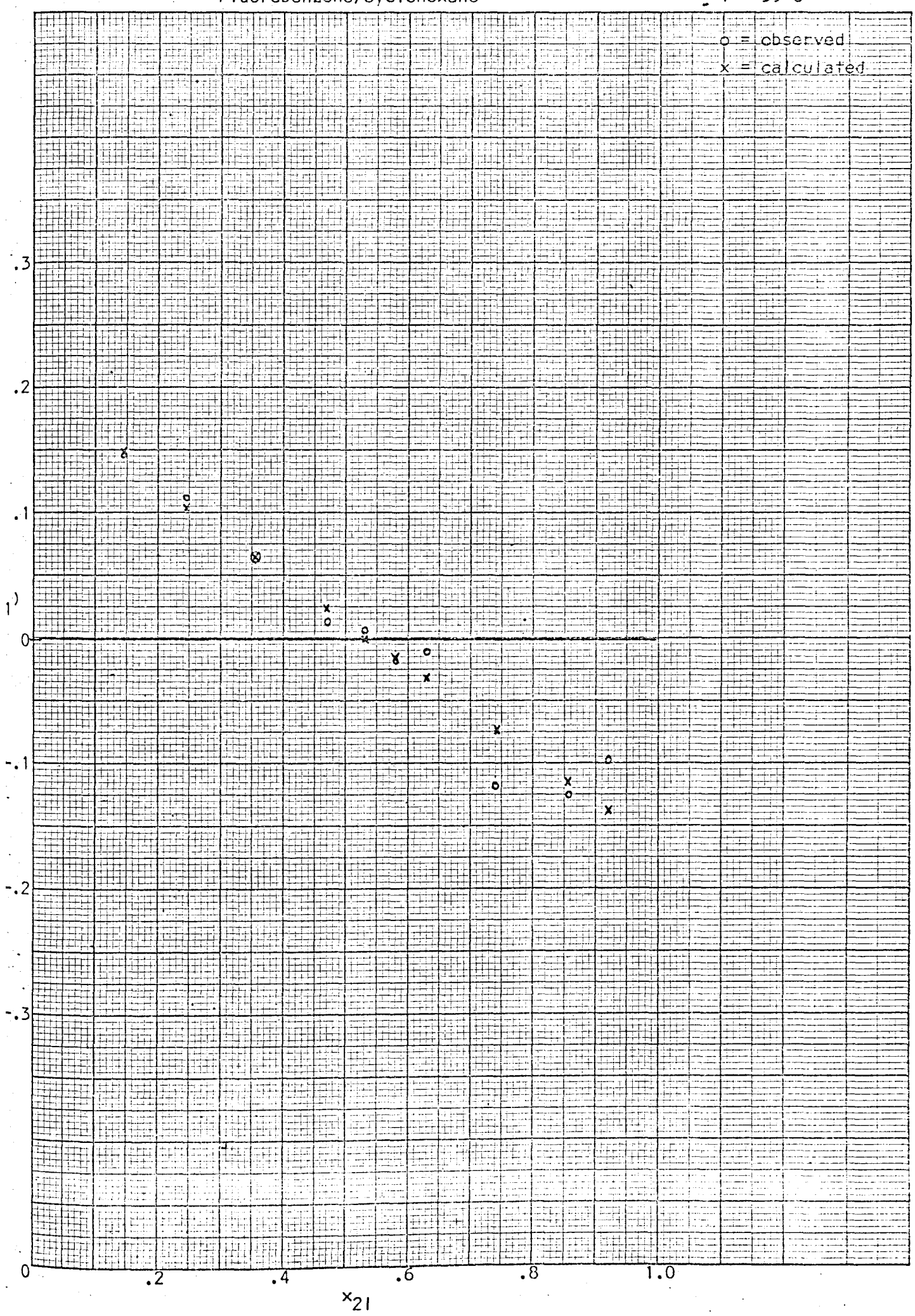
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	†	P_2 CALC.	DIF.
1	529.6478	22.0782	23.9896	335.8970	-1.9970
2	-374.8206	64.9325	-5.7725	311.5436	5.9226
3	181.0697	45.4052	3.9879	291.9733	-1.8132
				260.8570	-7.8220
Degrees of Freedom= 9				230.3980	6.4868
Confidence in First Term= 99.5%+				216.3378	1.0151
Confidence in Last Term= 99.5%				202.8618	0.4213
				184.7128	-1.3764
				149.3568	-1.1401
				110.3441	0.2952
				68.8948	-0.1772
				0.0000	0.0000

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	†	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1928	0.0192	10.0240	------	------
1	-0.3601	0.0322	-11.1978	-0.1391	0.0416
				-0.1150	-0.0109
Degrees of Freedom= 8				-0.0747	-0.0447
Integral at x=1: 0.0127				-0.0343	-0.0231
Error in integral: 0.0219				-0.0159	-0.0088
				0.0013	-0.0095
				0.0238	-0.0096
				0.0645	0.0025
				0.1042	0.0098
				0.1491	0.0065
				------	------


Fluorobenzene/Cyclohexane
T = 59°C
○ = observed
× = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x_{21}


Fluorobenzene/Cyclohexane
T = 59°C
o = observed
x = calculated
.3
.2
.1
0
-.1
-.2
-.3
0
.2
.4
.6
.8
1.0
x_{21}

System: Fluorobenzene/Cyclohexane T= 70°C.

Reference: Bhattacharyya,Anantaramav,Palit:Transaction Farad. Soc. 59,110(1963)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
474.02	1.0000	1.0000	474.0200	1.0000	1.0000	------
502.50	0.9241	0.8883	446.3707	1.0190	1.3626	-0.1262
493.35	0.8514	0.7907	390.0770	0.9665	1.2803	-0.1221
550.15	0.7352	0.6688	367.9458	1.0558	1.2673	-0.0793
567.55	0.6417	0.5876	333.5151	1.0964	1.2029	-0.0402
570.90	0.5782	0.5273	301.0242	1.0984	1.1782	-0.0305
573.89	0.5286	0.4930	282.9335	1.1292	1.1366	-0.0029
585.47	0.4709	0.4453	260.7039	1.1681	1.1303	0.0143
587.63	0.3721	0.3531	207.4628	1.1764	1.1149	0.0233
583.25	0.2458	0.2683	156.4626	1.3428	1.0421	0.1101
572.55	0.1427	0.1673	95.8048	1.4167	1.0241	0.1410
543.01	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	740.2209	42.7982	17.2956
2	-527.9058	125.5017	-4.2064
3	260.3799	57.5328	2.9747

Degrees of Freedom= 9
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.0%+

p_2 CALC.	DIF.
472.6949	1.3251
438.7220	-7.6487
408.2722	-18.1952
362.3511	5.5947
326.4217	7.0934
301.8326	-0.8085
282.2286	0.7049
258.6768	2.0271
215.7353	-8.2725
153.9236	2.5301
95.6120	0.19
0.0000	0.00

THERMODYNAMIC CONSISTENCY CURVE FITTING:

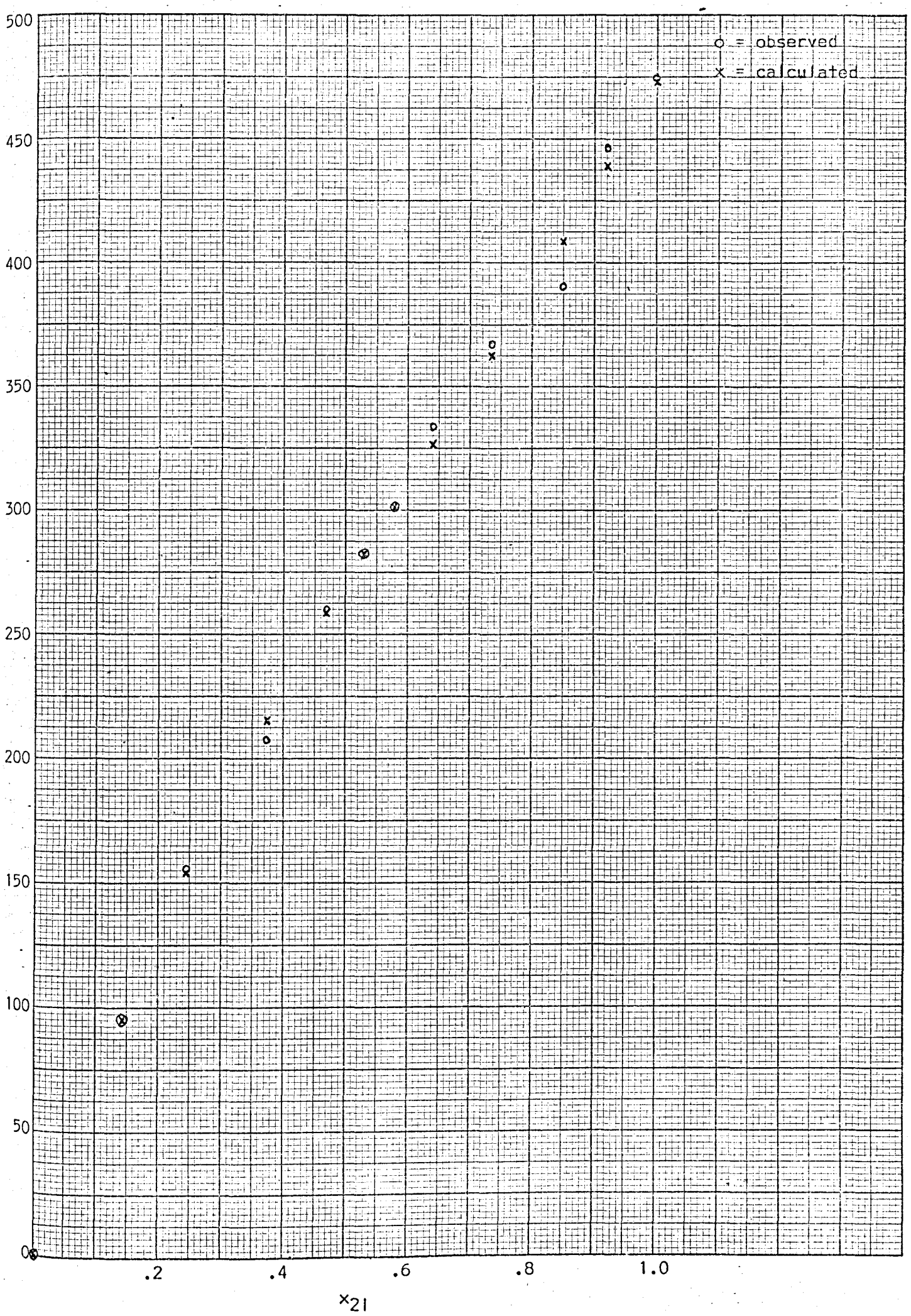
n	a_n	STD. ERROR	t
0	0.1805	0.0108	16.7508
1	-0.3493	0.0180	-19.4083

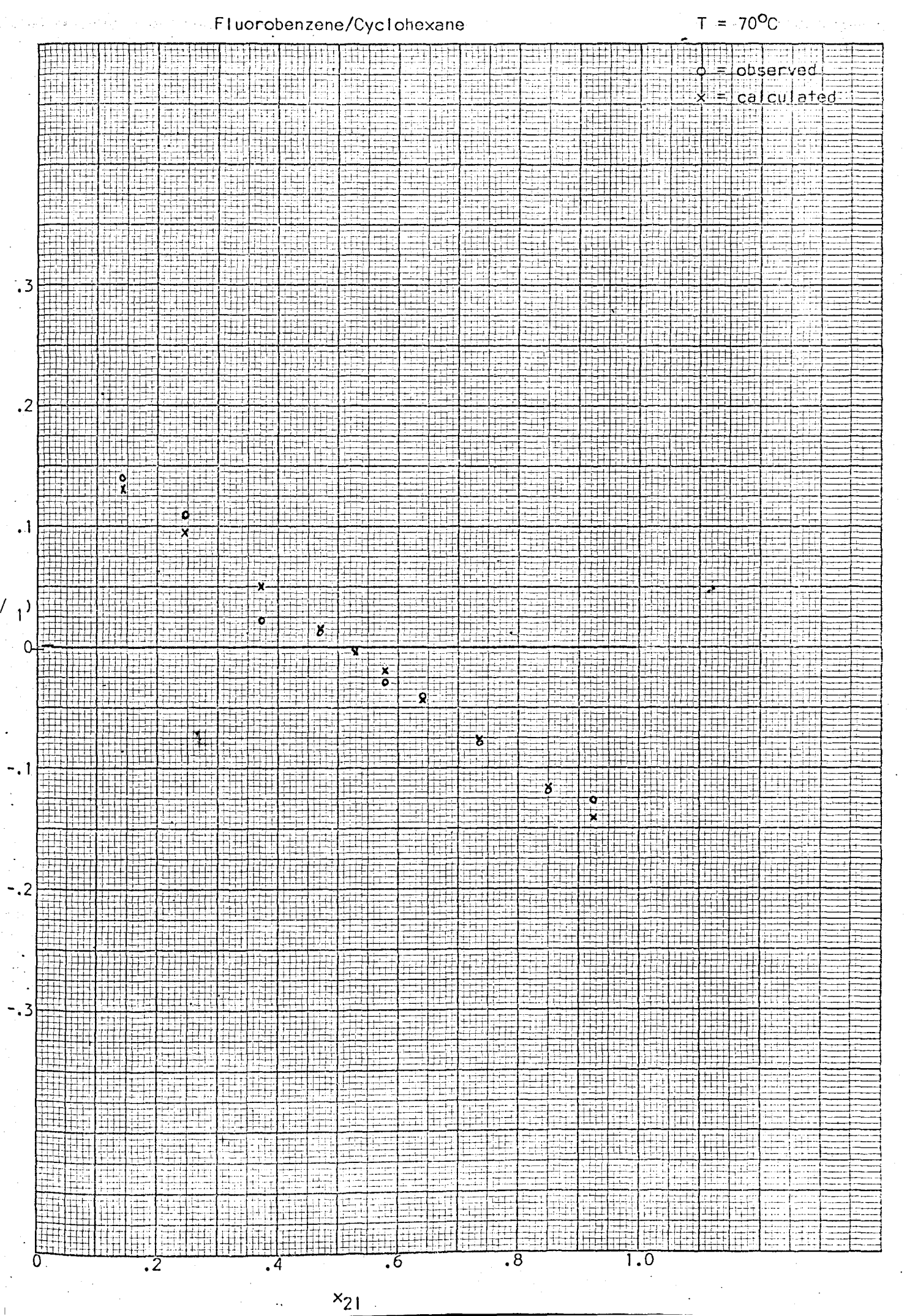
Degrees of Freedom= 8
Integral at x=1: 0.0059
Error in Integral: 0.0122

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
------	------
-0.1423	0.0160
-0.1169	-0.0052
-0.0763	-0.0030
-0.0436	0.0034
-0.0214	-0.0091
-0.0041	0.0013
0.0161	-0.0018
0.0506	-0.0273
0.0947	0.0154
0.1307	0.0103
------	------

Fluorobenzene/Cyclohexane

T = 70°C




Fluorobenzene/Cyclohexane
T = 70°C
o = observed
x = calculated
.3
.2
.1
0
-.1
-.2
-.3
0
.2
.4
.6
.8
1.0
x21

System: Cyclohexane/Benzene T= 40°C.

Reference: Scatchard G.,Wood S.E.,Mochel J.M.:J.Phys.Chem,43, 119(1939)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
194.94	0.8718	0.8343	162.6384	0.9913	1.3402	-0.1310
200.65	0.7646	0.7234	145.1502	1.0087	1.2541	-0.0946
204.75	0.6315	0.6088	124.6518	1.0488	1.1562	-0.0423
206.12	0.5068	0.5050	104.0906	1.0913	1.1004	-0.0036
205.18	0.3857	0.4091	83.9391	1.1564	1.0498	0.0420
201.73	0.2572	0.3021	60.9426	1.2590	1.0082	0.0965
195.04	0.1344	0.1795	35.0097	1.3841	0.9834	0.1484

PARTIAL PRESSURE CURVE FITTING:

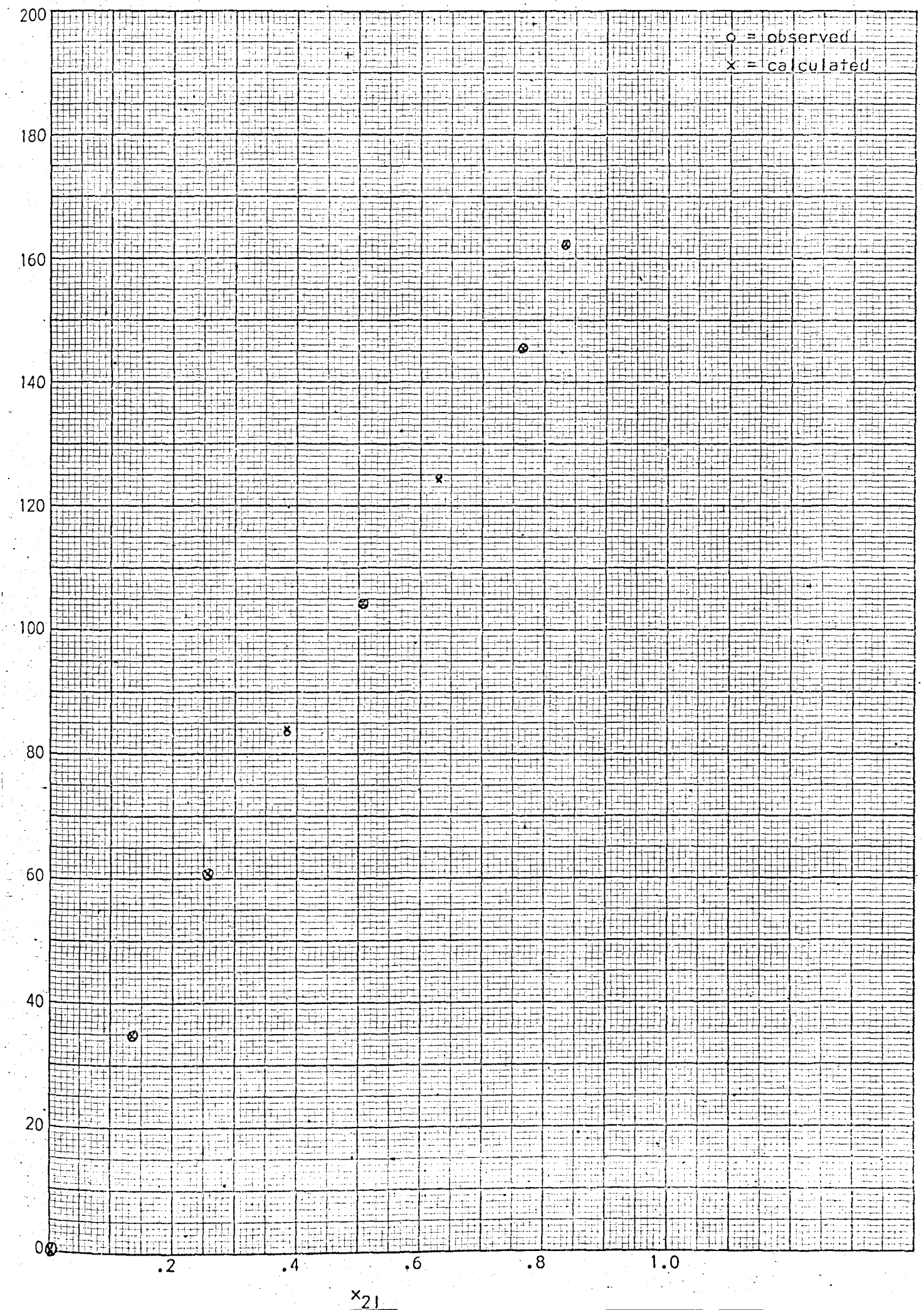
n	a_n	STD.ERROR	†	P_2 CALC.	DIF.
1	294.7422	4.3707	67.4365	162.5382	0.1002
2	-291.3554	26.1133	-11.1573	145.4815	-0.3313
3	278.3307	48.5084	5.7378	124.2308	0.4210
4	-99.3662	28.1430	-3.5308	104.2168	-0.1262
				84.1099	-0.1707
				60.8348	0.1079
				34.9938	0.0159

Degrees of Freedom= 4
Confidence in First Term= 99.5%+
Confidence in Last Term= 97.5%+

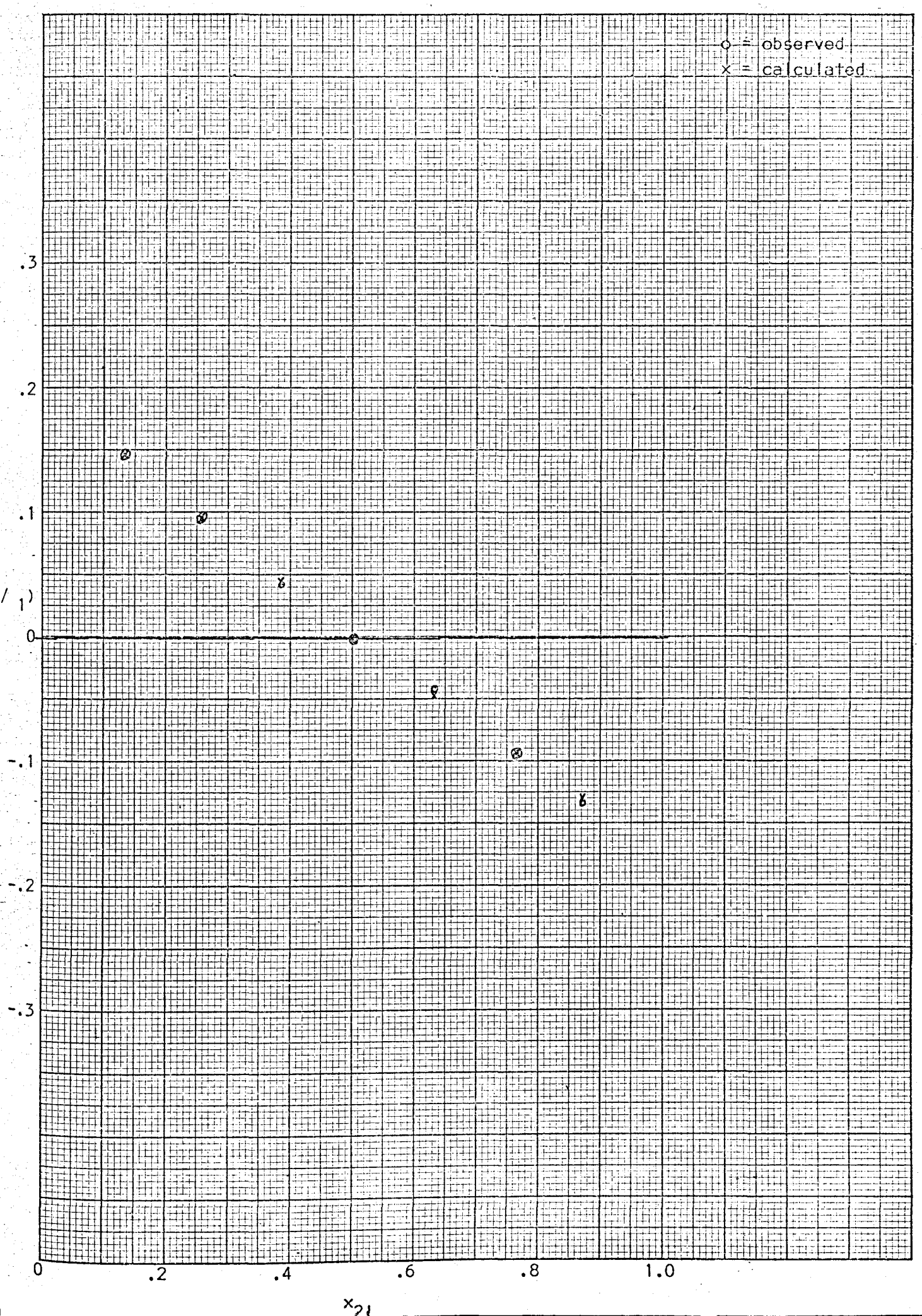
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	†	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.2059	0.0052	39.4047	-0.1298	-0.0012
1	-0.4436	0.0237	-18.6991	-0.0940	-0.0005
2	0.0671	0.0230	2.9179	-0.0475	0.0052
				-0.0017	-0.0019
				0.0448	-0.0028
				0.0962	0.0003
				0.1475	0.0010

Degrees of Freedom= 4
Integral at x=1: 0.0065
Error in Integral: 0.0025


Cyclohexane/Benzene
T = 40°C
o = observed
x = calculated
200
180
160
140
120
100
80
60
40
20
0
.2
.4
.6
.8
1.0
x_{21}

Cyclohexane/Benzene T = 40°C



System: Cyclohexane/Benzene T= 70°C.

Reference: Scatchard G.,Wood S.E.,Mochel J.M.:J.Phys. Chem,43, 119(1939)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
567.60	0.8814	0.8514	483.2546	0.9983	1.2722	-0.1053
584.90	0.7591	0.7195	420.8355	1.0093	1.2183	-0.0817
596.16	0.6241	0.6018	358.7691	1.0467	1.1297	-0.0331
600.27	0.5055	0.5025	301.6357	1.0865	1.0803	0.0025
599.32	0.3820	0.3973	238.1098	1.1350	1.0456	0.0356
593.48	0.2752	0.3038	180.2992	1.1929	1.0198	0.0681
577.79	0.1341	0.1689	97.5887	1.3251	0.9921	0.1257

PARTIAL PRESSURE CURVE FITTING:

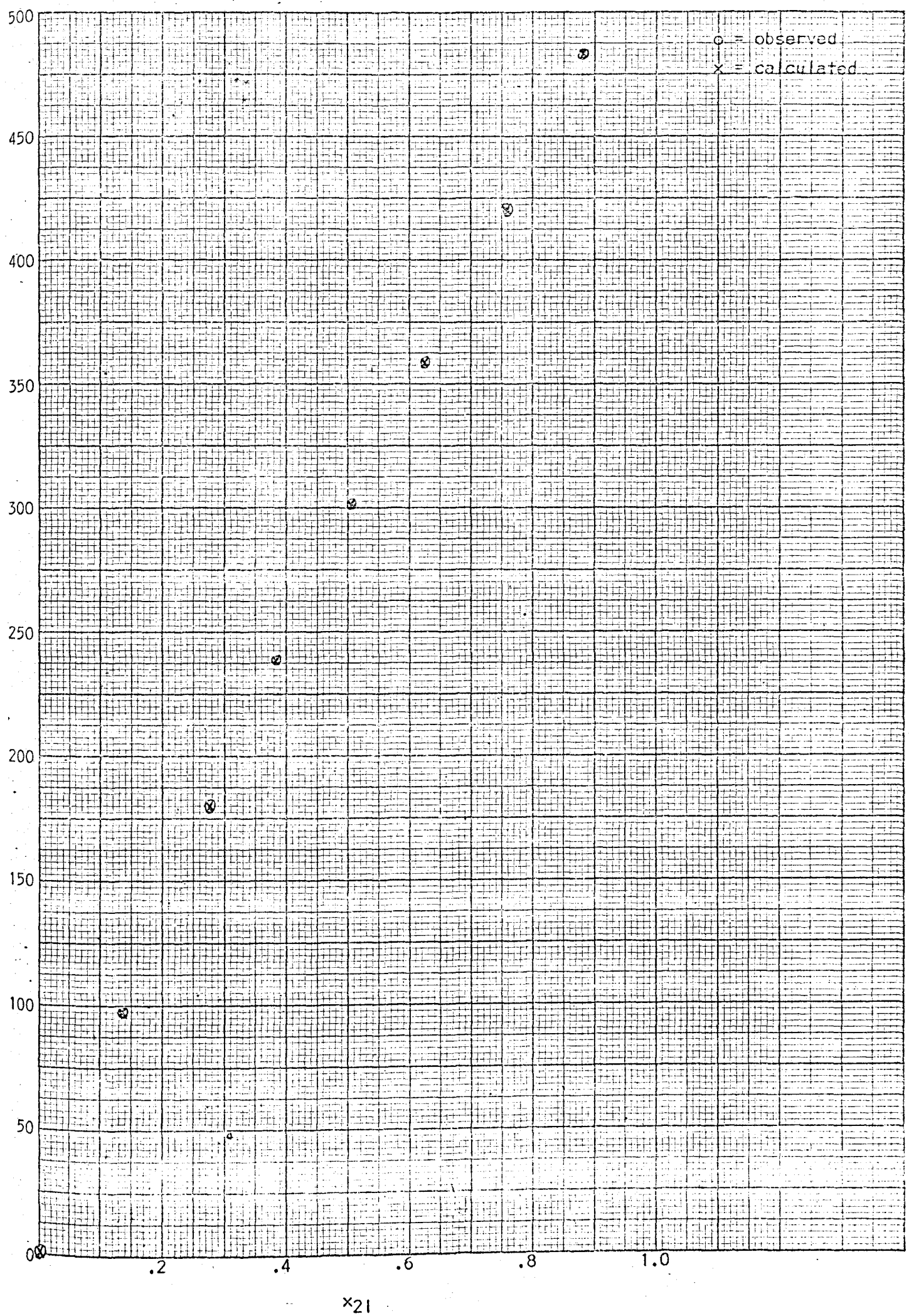
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	857.9273	0.2707	3169.0482	483.2547	-0.0001
2	-1290.0875	2.4393	-528.8656	420.8356	-0.0001
3	2781.1095	7.5991	365.9768	358.7668	0.0023
4	-3185.6291	9.7654	-326.2157	301.6431	-0.0074
5	1405.3902	4.4213	317.8692	238.0984	0.0115
				180.3077	-0.0085
				97.5861	0.0027

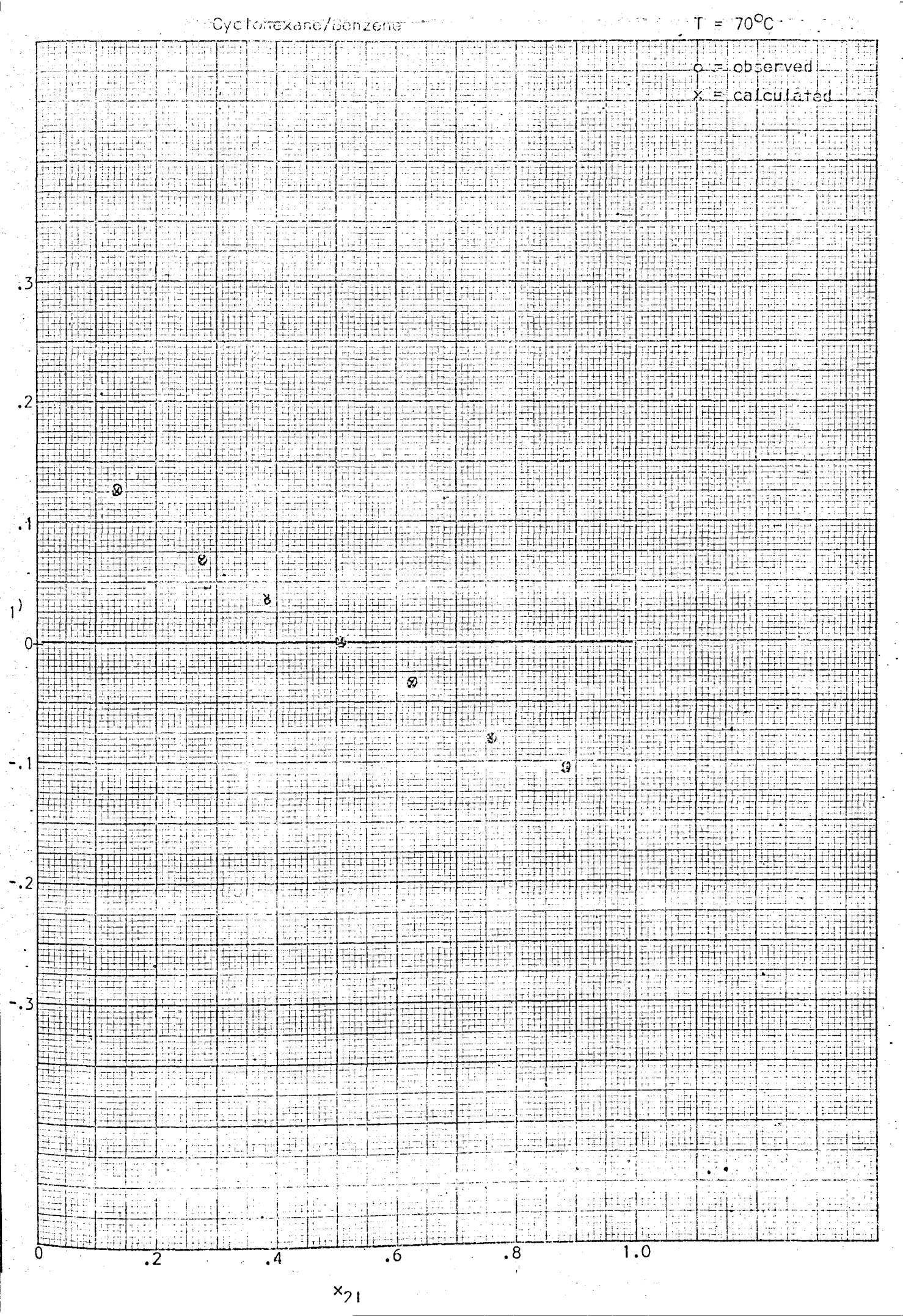
Degrees of Freedom= 3
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.2396	0.0161	14.8943	-0.1057	0.0004
1	-1.1786	0.1848	-6.3785	-0.0802	-0.0014
2	2.9881	0.6731	4.4392	-0.0352	0.0021
3	-4.1428	0.9655	-4.2910	0.0031	-0.0006
4	2.0031	0.4743	4.2236	0.0372	-0.0015
				0.0667	0.0014
				0.1260	-0.0003

Degrees of Freedom= 2
Integral at x=1: 0.0113
Error in Integral: 0.0014


Cyclohexane/Benzene
T = 70°C
o = observed
x = calculated
500
450
400
350
300
250
200
150
100
50
0
.2
.4
.6
.8
1.0
x21


Cyclohexane/benzene
T = 70°C
o = observed
x = calculated
.3
.2
.1
0
-.1
-.2
-.3
1)
0
.2
.4
.6
.8
1.0
x21

System: Chloroform/Carbon Tetrachloride T= 40°C.

Reference: McGlashan M.L.,Prue J.E.,Sainsbury J.E.J.:Trans.Farad. Soc. 50,1284(1954)

P_{12}	x_{2l}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
220.25	0.0319	0.0614	13.5233	1.1766	0.9969	0.0720
220.23	0.0322	0.0589	12.9715	1.1181	0.9998	0.0486
229.76	0.0806	0.1448	33.2692	1.1456	0.9977	0.0600
230.07	0.0827	0.1466	33.7283	1.1319	0.9993	0.0541
248.71	0.1840	0.2936	73.0213	1.1015	1.0052	0.0397
269.47	0.3074	0.4401	118.5937	1.0708	1.0170	0.0224
269.81	0.3108	0.4424	119.3639	1.0659	1.0191	0.0195
286.98	0.4218	0.5560	159.5609	1.0499	1.0288	0.0088
287.35	0.4241	0.5594	160.7436	1.0520	1.0263	0.0107
287.89	0.4279	0.5608	161.4487	1.0472	1.0318	0.0064
301.34	0.5200	0.6428	193.7014	1.0339	1.0469	-0.0054
301.84	0.5242	0.6456	194.8679	1.0318	1.0496	-0.0074
315.51	0.6258	0.7288	229.9437	1.0198	1.0675	-0.0199
315.72	0.6268	0.7302	230.5387	1.0208	1.0656	-0.0186
328.52	0.7266	0.8038	264.0644	1.0087	1.1006	-0.0379
328.98	0.7283	0.8056	265.0263	1.0100	1.0989	-0.0366
343.00	0.8438	0.8887	304.8241	1.0026	1.1410	-0.0561
342.84	0.8449	0.8895	304.9562	1.0018	1.1403	-0.0562
351.26	0.9145	0.9395	330.0088	1.0016	1.1604	-0.0639
351.33	0.9152	0.9401	330.2853	1.0016	1.1586	-0.0632
352.81	0.9273	0.9483	334.5697	1.0014	1.1713	-0.0681
356.28	0.9599	0.9708	345.8766	1.0001	1.2112	-0.0832

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	416.1219	1.2463	333.8796
2	-115.6201	3.8501	-30.0303
3	60.1227	2.8124	21.3776

Degrees of Freedom= 20
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

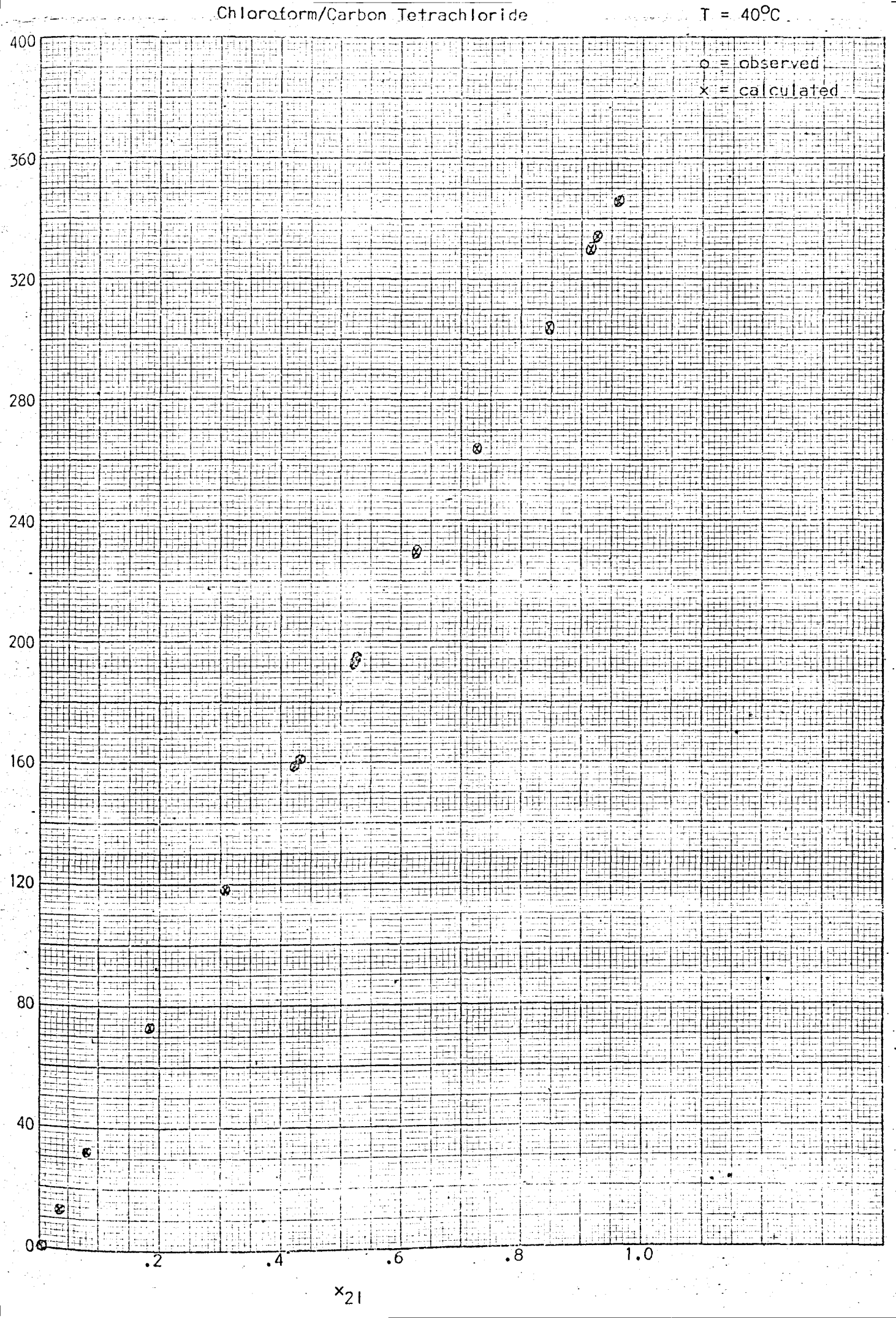
P_2 CALC.	DIF.
13.1586	0.3648
13.2813	-0.3097
32.8198	0.4495
33.6565	0.0717
73.0265	-0.0053
118.7368	-0.1431
119.9672	-0.6032
159.4615	0.0994
160.2679	0.4757
161.5992	-0.1505
193.5734	0.1279
195.0206	-0.1527
229.8641	0.0796
230.2062	0.3326
264.3763	-0.3119
264.9600	0.0663
304.9231	-0.0990
305.3075	-0.3513
329.8313	0.1774
330.0802	0.2051
334.3899	0.1798
346.0782	-0.2016

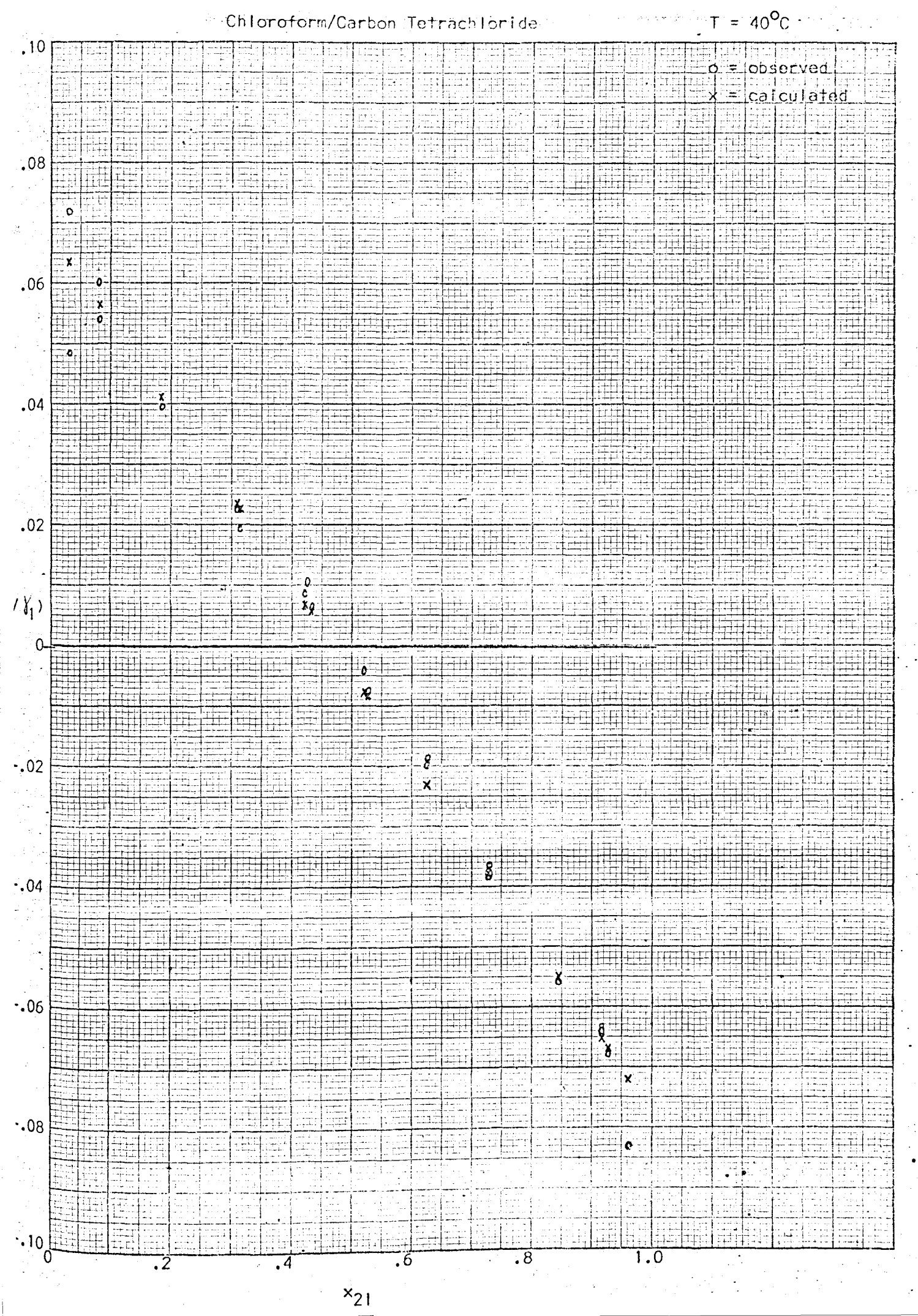
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.0682	0.0022	31.6566
1	-0.1461	0.0036	-41.0333

Degrees of Freedom= 20
Integral at x=1: -0.0049
Error in Integral: 0.0049

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0.0635	0.0084
0.0635	-0.0149
0.0564	0.0036
0.0561	-0.0020
0.0413	-0.0016
0.0233	-0.0009
0.0228	-0.0033
0.0066	0.0023
0.0062	0.0045
0.0057	0.0008
-0.0078	0.0023
-0.0084	0.0010
-0.0232	0.0034
-0.0234	0.0048
-0.0380	0.0001
-0.0382	0.0016
-0.0551	-0.0010
-0.0553	-0.0010
-0.0654	0.0015
-0.0655	0.0023
-0.0673	-0.0008
-0.0721	-0.0111


Chloroform/Carbon Tetrachloride
T = 40°C
o = observed
x = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x_{21}


Chloroform/Carbon Tetrachloride
T = 40°C
o = observed
x = calculated
.10
.08
.06
.04
.02
0
-.02
-.04
-.06
-.08
-.10
(γ1)
0
.2
.4
.6
.8
1.0
x21

System: Chloroform/Carbon Tetrachloride T= 55°C.

Reference: McGlashan M.L.,Prue J.E.,Sainsbury J.E.J.:Trans.Farad. Soc, 50,1284(1954)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
380.86	0.0227	0.0424	16.1485	1.1530	0.9978	0.0628
382.46	0.0281	0.0497	19.0083	1.0964	0.9999	0.0400
386.02	0.0394	0.0691	26.6740	1.0973	1.0002	0.0402
389.74	0.0502	0.0871	33.9464	1.0960	1.0016	0.0391
392.78	0.0597	0.1035	40.6527	1.1036	1.0013	0.0423
422.66	0.1592	0.2505	105.8763	1.0779	1.0074	0.0294
430.97	0.1840	0.2868	123.6022	1.0887	1.0072	0.0338
475.71	0.3516	0.4786	227.6748	1.0495	1.0228	0.0112
491.04	0.4118	0.5398	265.0634	1.0432	1.0272	0.0067
496.09	0.4313	0.5557	275.6772	1.0359	1.0363	-0.0001
508.76	0.4819	0.6033	306.9349	1.0323	1.0416	-0.0039
512.78	0.4994	0.6184	317.1032	1.0291	1.0451	-0.0067
523.10	0.5420	0.6584	344.4090	1.0299	1.0432	-0.0056
526.17	0.5520	0.6677	351.3237	1.0315	1.0435	-0.0050
551.34	0.6700	0.7578	417.8055	1.0107	1.0820	-0.0296
563.01	0.7209	0.7990	449.8450	1.0114	1.0841	-0.0302
564.14	0.7272	0.8017	452.2710	1.0080	1.0965	-0.0365
503.63	0.9199	0.9418	568.4987	1.0016	1.1727	-0.0685
604.27	0.9222	0.9457	571.4581	1.0043	1.1277	-0.0503
613.76	0.9730	0.9822	602.8351	1.0042	1.0819	-0.0324

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	†
1	692.8820	4.3178	160.4700
2	-154.0900	13.1472	-11.7204
3	80.2828	9.4344	8.5096

Degrees of Freedom= 18
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

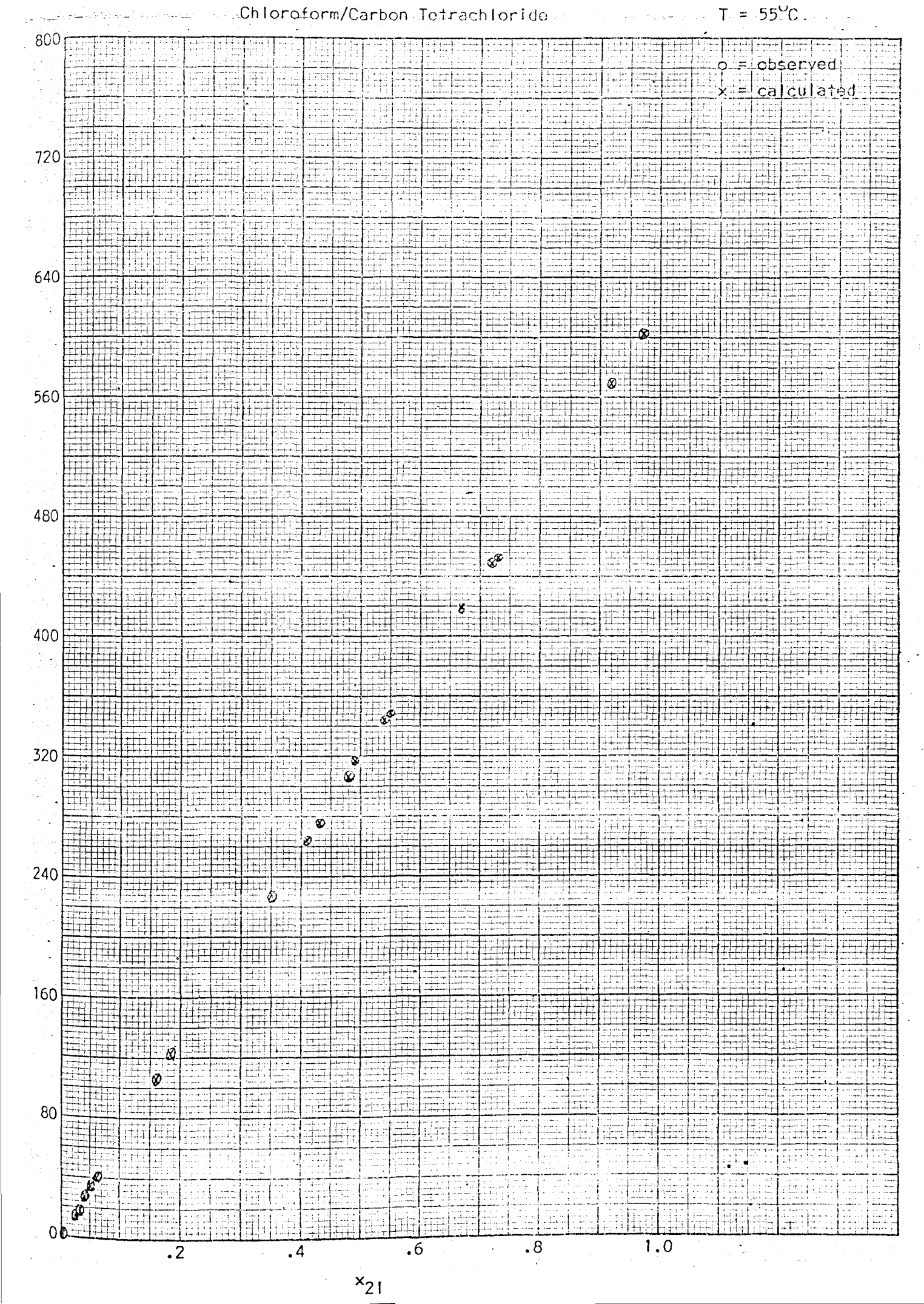
P_2 CALC.	DIF.
15.6500	0.4985
19.3501	-0.3418
27.0653	-0.3913
34.4045	-0.4582
40.8329	-0.1802
106.7254	-0.8491
122.7735	0.8287
228.0579	-0.3831
264.8047	0.2587
276.6174	-0.9401
307.1004	-0.1655
317.5944	-0.4913
343.0586	1.3505
349.0223	2.3014
419.2060	-1.4006
449.4965	0.3485
453.2513	-0.9803
569.4836	-0.9849
570.8943	0.5638
602.2466	0.5885

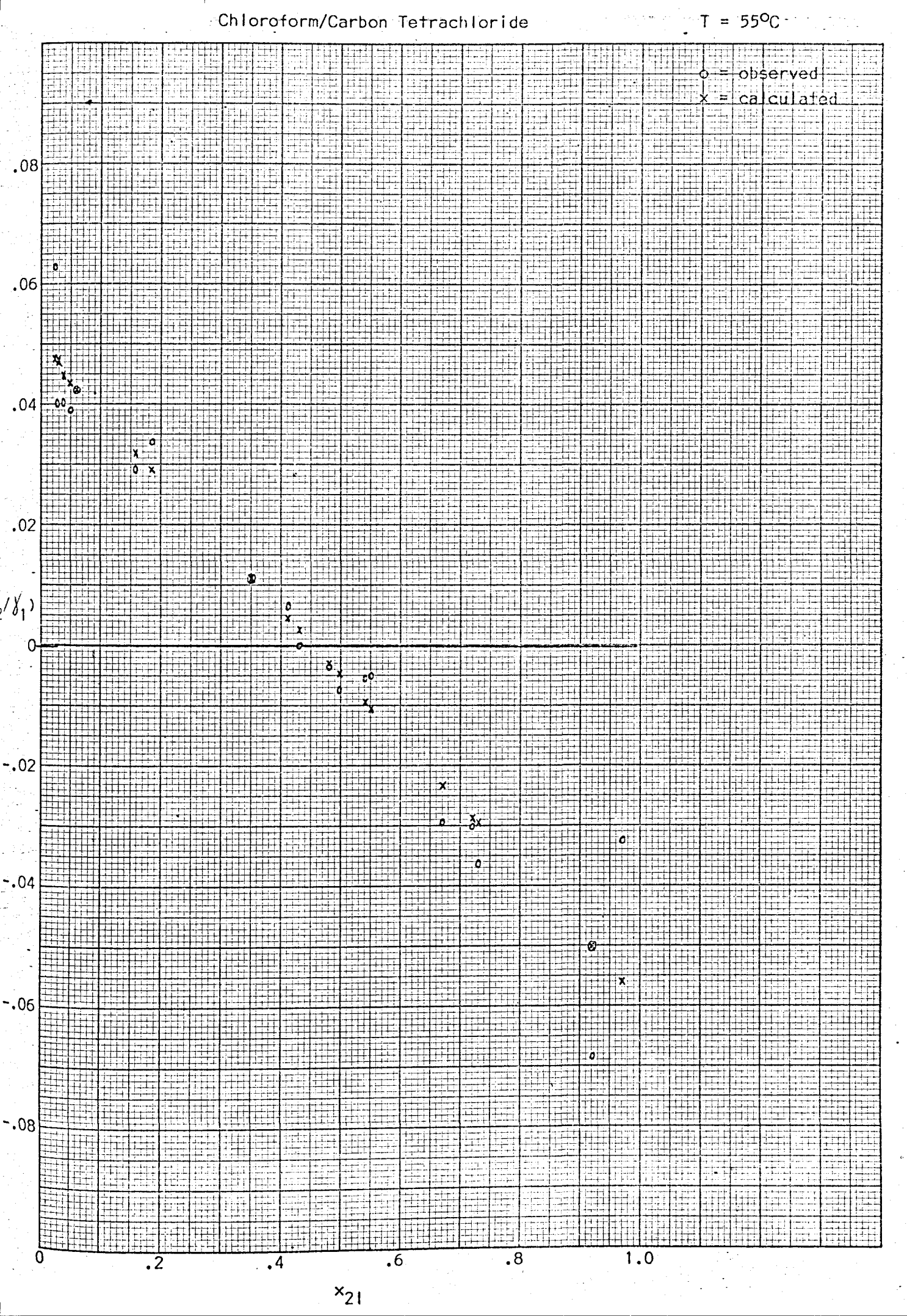
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.0491	0.0034	14.3941
1	-0.1080	0.0063	-17.0166

Degrees of Freedom= 18
Integral at x=1: -0.0049
Error in Integral: 0.0266

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0.0466	0.0161
0.0460	-0.0060
0.0448	-0.0046
0.0436	-0.0045
0.0426	-0.0004
0.0319	-0.0025
0.0292	0.0046
0.0111	0.0001
0.0046	0.0021
0.0025	-0.0026
-0.0030	-0.0009
-0.0049	-0.0018
-0.0095	0.0039
-0.0106	0.0055
-0.0233	-0.0063
-0.0288	-0.0014
-0.0295	-0.0070
-0.0503	-0.0182
-0.0505	0.0002
-0.0560	0.0237


Chloroform/Carbon Tetrachloride
T = 55°C.
o = observed
x = calculated
800
720
640
560
480
400
320
240
160
80
0
.2
.4
.6
.8
1.0
x_{21}


Chloroform/Carbon Tetrachloride
T = 55°C
o = observed
x = calculated
.08
.06
.04
.02
0
-.02
-.04
-.06
-.08
0
.2
.4
.6
.8
1.0
x_{21}

System: Carbon Tetrachloride/Benzene T = 40°C

Reference: Fowler R.T.,Lim S.C.:J.Apll.Chem.,6,74(1956)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
185.00	0.0994	0.1244	23.0140	1.0983	0.9954	0.0427
189.00	0.1858	0.2233	42.2037	1.0775	0.9978	0.0334
195.00	0.3401	0.3824	74.5680	1.0401	1.0100	0.0128
198.00	0.4393	0.4815	95.3370	1.0295	1.0133	0.0069
201.00	0.5324	0.5681	114.1881	1.0174	1.0274	-0.0042
203.00	0.6063	0.6363	129.1689	1.0106	1.0378	-0.0115
205.00	0.6815	0.7043	144.3815	1.0050	1.0533	-0.0204
207.00	0.7812	0.7964	164.8548	1.0011	1.0660	-0.0273
209.00	0.8926	0.8990	187.8910	0.9986	1.0877	-0.0371
210.00	0.9529	0.9555	200.6550	0.9989	1.0980	-0.0411
210.00	0.9632	0.9653	202.7130	0.9984	1.0958	-0.0404

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	237.9056	1.1908	199.7879
2	-70.9113	6.3628	-11.1447
3	57.9568	10.7358	5.3985
4	-14.4044	5.6706	-2.5402

Degrees of Freedom= 8
Confidence in First Term= 99.5%+
Confidence in Last Term= 97.5%+

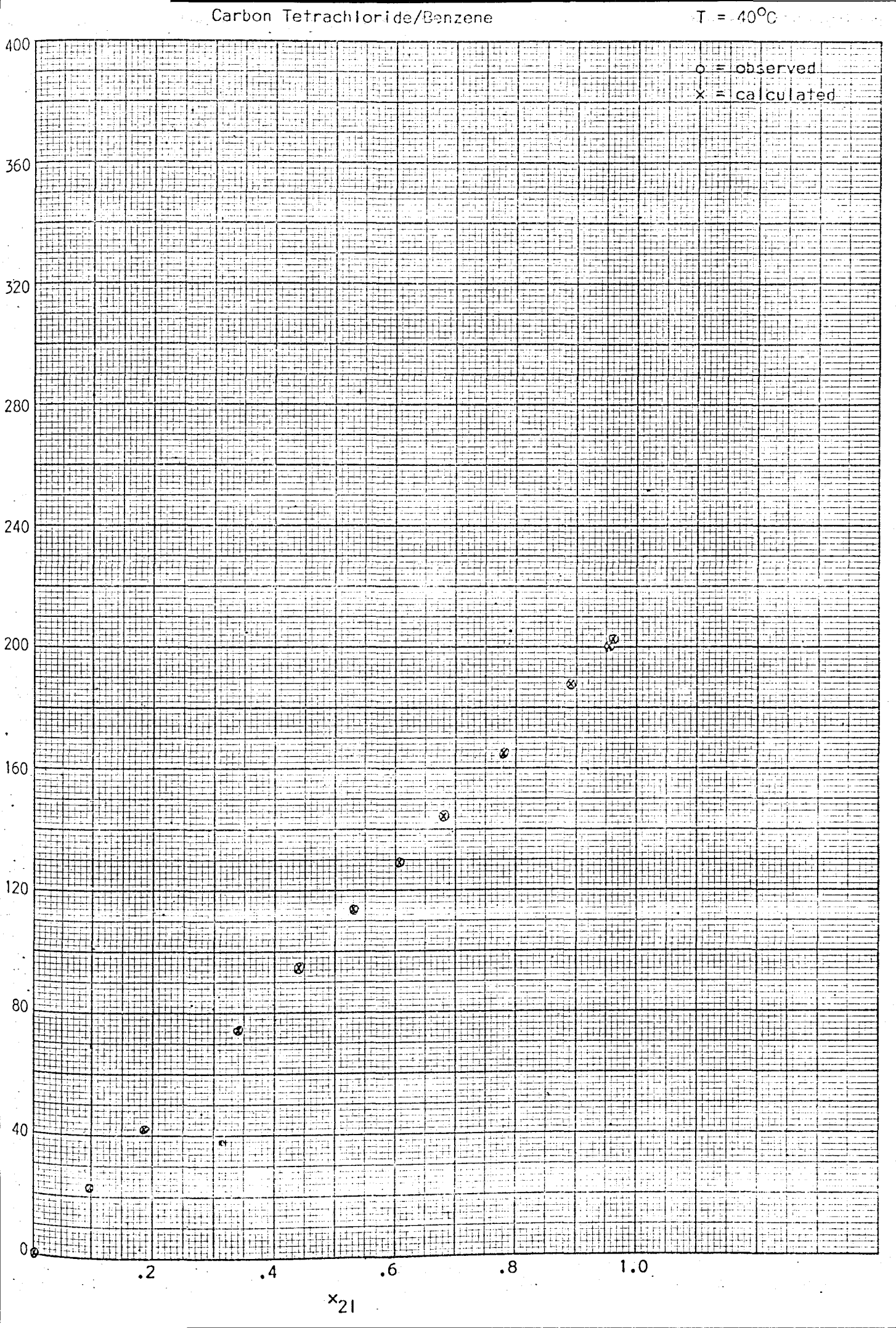
P_2 CALC.	DIF.
23.0027	0.0113
42.1095	0.0942
74.7967	-0.2287
95.2041	0.1329
114.1500	0.0281
129.1459	0.0230
144.4357	-0.0542
164.8425	0.0123
187.9302	-0.0392
200.5822	0.0728
202.7551	-0.0421

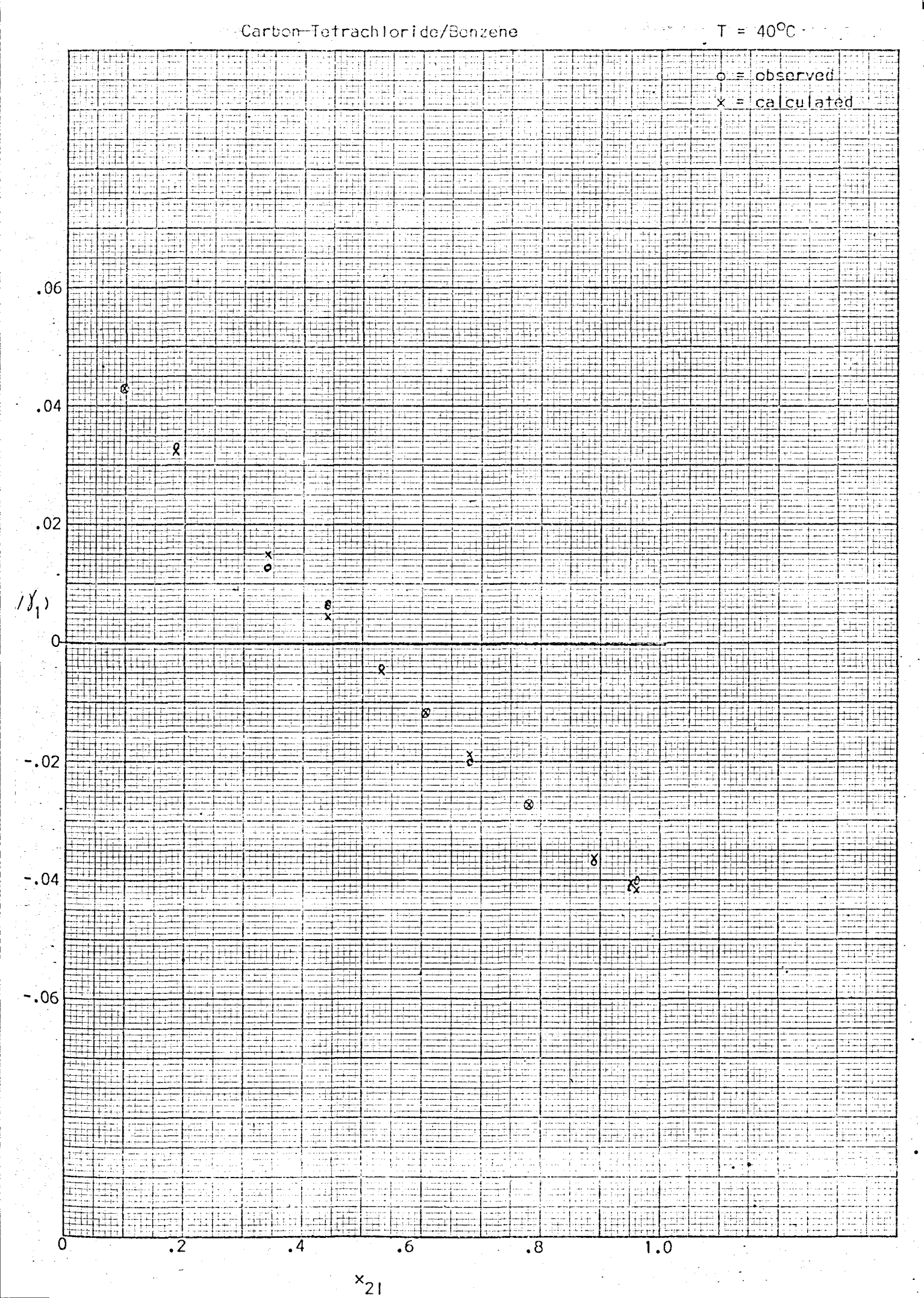
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.0556	0.0017	33.1837
1	-0.1290	0.0069	-18.7979
2	0.0292	0.0061	4.8271

Degrees of Freedom= 8
Integral at x=1: 0.0008
Error in Integral: 0.0012

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0.0431	-0.0003
0.0326	0.0008
0.0151	-0.0023
0.0046	0.0023
-0.0048	0.0006
-0.0119	0.0004
-0.0188	-0.0016
-0.0274	0.0001
-0.0363	-0.0008
-0.0408	-0.0002
-0.0416	0.0011


Carbon Tetrachloride/Benzene
T = 40°C
o = observed
x = calculated
400
360
320
280
240
200
160
120
80
40
0
.2
.4
.6
.8
1.0
x21


Carbon-Tetrachloride/Benzene
T = 40°C
o = observed
x = calculated
.06
.04
.02
0
-.02
-.04
-.06
/γ1)
0
.2
.4
.6
.8
1.0
x21

System: Carbon Tetrachloride/Benzene T= 40°C.

Reference: Scatchard G.,Wood S.E.,Mochel J.M.:J.Am.Chem.Soc. 62,712(1940)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
190.18	0.1398	0.1703	32.3877	1.0861	2.1864	-0.3038
194.70	0.2378	0.2774	54.0098	1.0648	2.2001	-0.3151
200.07	0.3735	0.4159	83.2091	1.0445	2.2232	-0.3280
204.02	0.4919	0.5295	108.0286	1.0296	2.2518	-0.3398
204.20	0.4986	0.5359	109.4308	1.0290	2.2528	-0.3403
207.44	0.6201	0.6475	134.3174	1.0155	2.2941	-0.3539
210.37	0.7585	0.7739	162.8053	1.0063	2.3475	-0.3678
211.97	0.8718	0.8783	186.1733	1.0012	2.3984	-0.3793

PARTIAL PRESSURE CURVE FITTING:

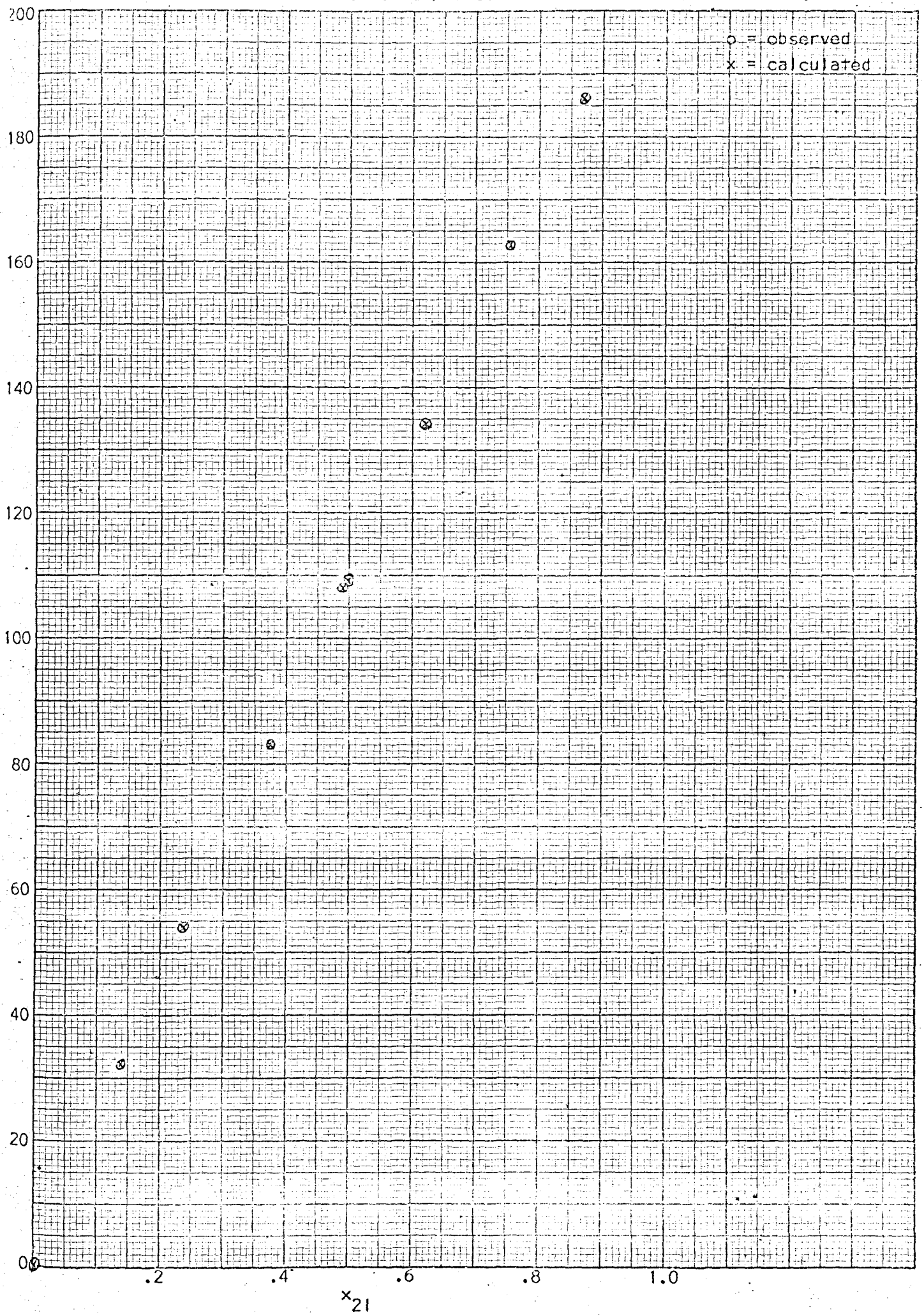
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	246.0649	1.1533	213.3602	32.3935	-0.0058
2	-159.0584	14.5126	-10.9600	53.9958	0.0140
3	534.3425	66.2912	8.0605	83.2300	-0.0209
4	-1076.7648	140.2467	-7.6776	108.0268	0.0018
5	1058.5878	139.2364	7.6028	109.4114	0.0194
6	-393.1701	52.4064	-7.5023	134.3296	-0.0122
				162.8016	0.0038
				186.1739	-0.0007

Degrees of Freedom= 3
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

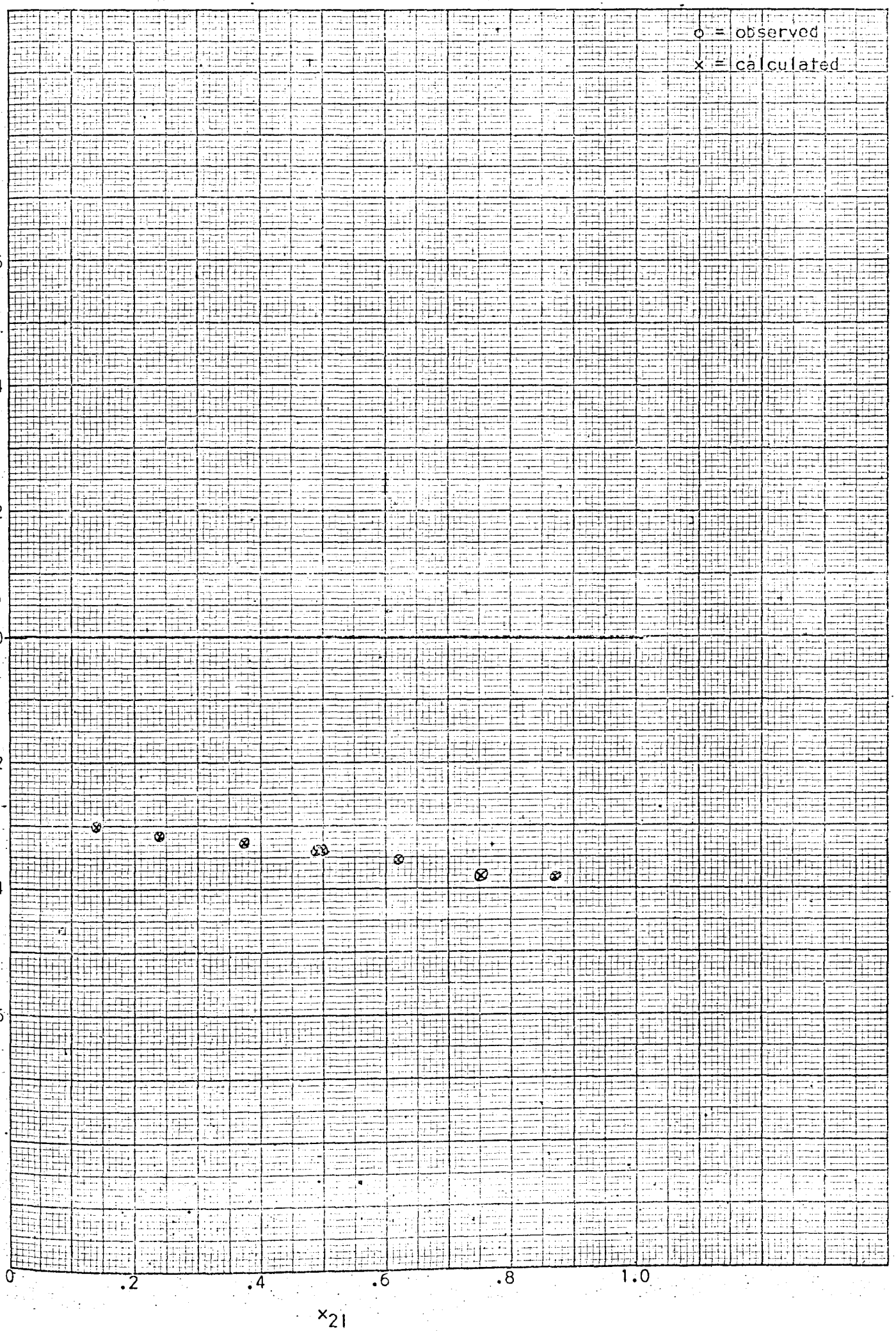
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	-0.2713	0.0050	-54.4461	-0.3038	0.0000
1	-0.3570	0.0712	-5.0110	-0.3152	0.0001
2	1.1998	0.3609	3.3246	-0.3278	-0.0002
3	-2.5319	0.8289	-3.0546	-0.3398	0.0000
4	2.4576	0.8781	2.7988	-0.3405	0.0003
5	-0.8951	0.3481	-2.5711	-0.3537	-0.0002
				-0.3679	0.0001
				-0.3793	0.0000

Degrees of Freedom= 2
Integral at x=1: -0.3405
Error in Integral: 0.0002


Carbon Tetrachloride/Benzene
T = 40°C
o = observed
x = calculated
200
180
160
140
120
100
80
60
40
20
0
.2
.4
.6
.8
1.0
x21

Carbon Tetrachloride/Benzene T = 40°C



System: Carbon Tetrachloride/Benzene T= 70°C.

Reference: Scatchard G.,Wood S.E.,Mochel J.M.:J.Am.Chem.Soc. 62,712(1940)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
568.89	0.1428	0.1666	94.7771	1.0688	0.9948	0.0312
579.13	0.2394	0.2702	156.4809	1.0526	0.9994	0.0225
591.62	0.3791	0.4105	242.8600	1.0316	1.0103	0.0091
600.77	0.4930	0.5304	312.6407	1.0212	1.0221	-0.0004
599.67	0.4939	0.5215	312.7279	1.0196	1.0197	0.0000
607.22	0.6224	0.6411	389.2887	1.0072	1.0380	-0.0131
613.08	0.7624	0.7719	473.2365	0.9995	1.0586	-0.0249
616.20	0.8750	0.8780	540.8656	0.9954	1.0814	-0.0360

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	680.4895	1.7999	378.0625
2	-127.7375	6.0338	-21.1703
3	64.5400	4.7908	13.4716

Degrees of Freedom= 6
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

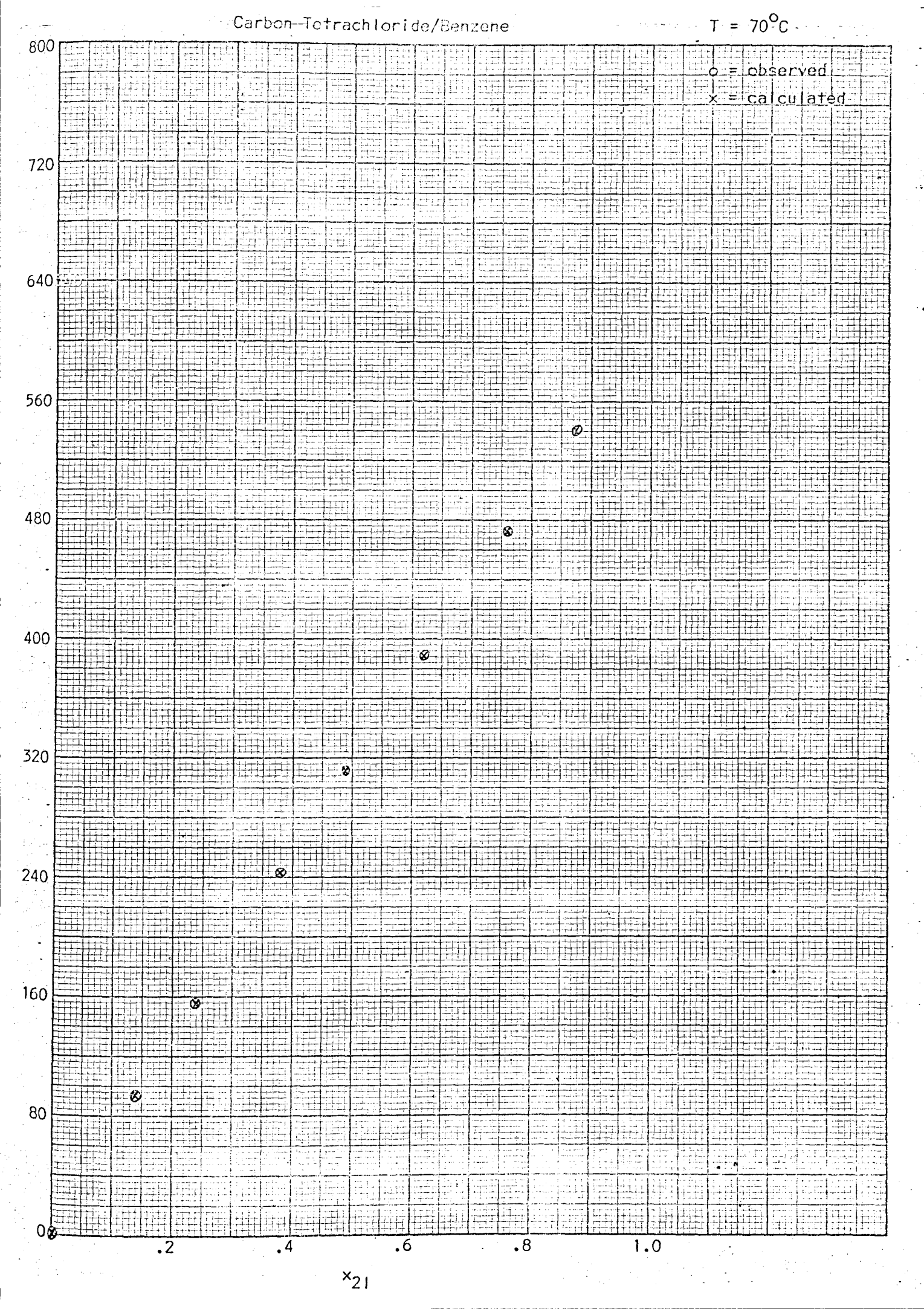
P_2 CALC.	DIF.
94.7570	0.0200
156.4738	0.0072
243.1319	-0.2719
312.1682	0.4725
312.7097	0.0183
389.6145	-0.3258
473.1581	0.0784
540.8661	-0.0005

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.0443	0.0004	100.1739
1	-0.0913	0.0008	-114.1348

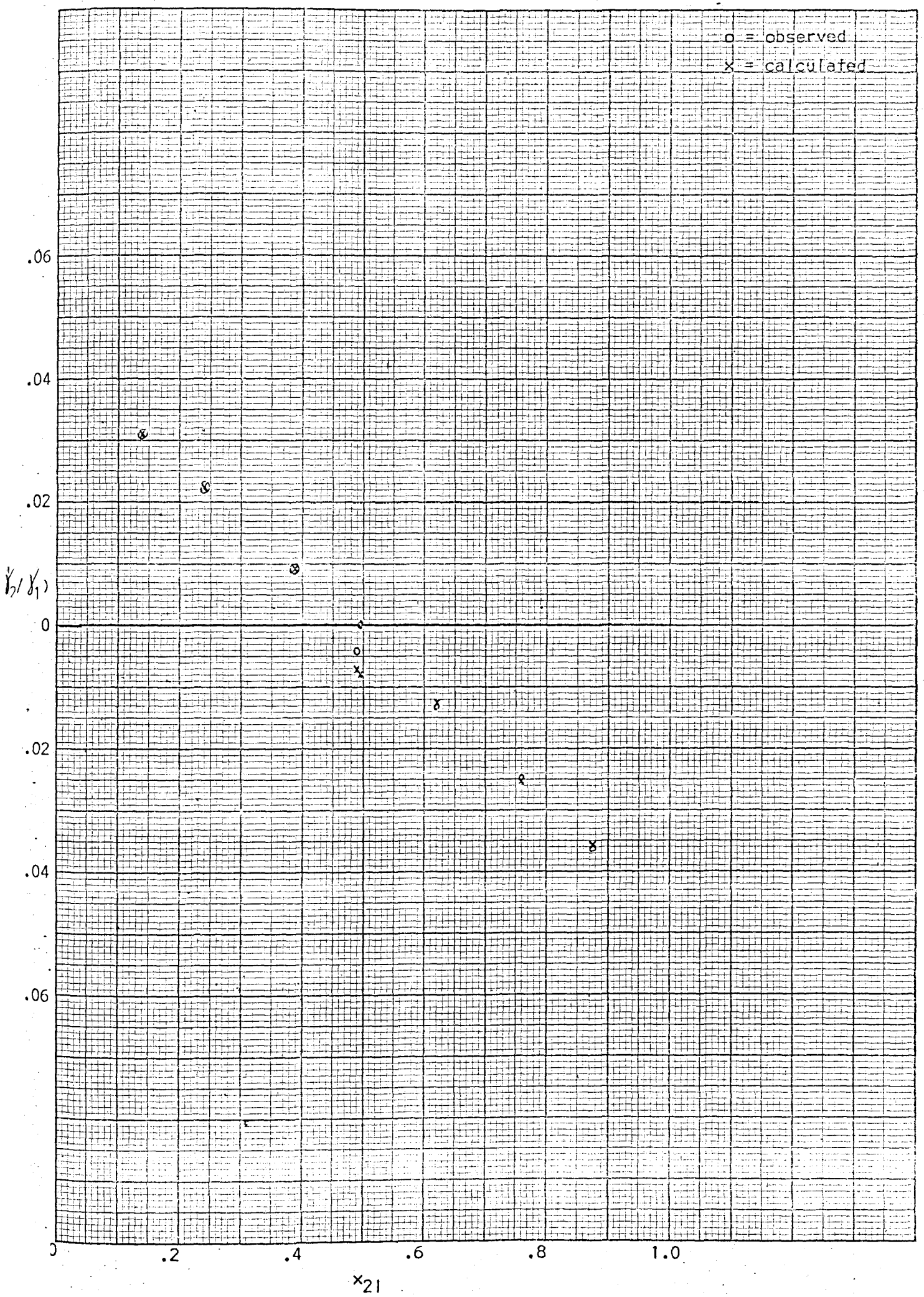
Degrees of Freedom= 6
Integral at x=1: -0.0014
Error in Integral: 0.0004

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0.0313	-0.0001
0.0224	0.0001
0.0097	-0.0006
-0.0007	0.0003
-0.0008	0.0008
-0.0126	-0.0005
-0.0253	0.0004
-0.0356	-0.0003


Carbon–Tetrachloride/Benzene
T = 70°C
o = observed
x = calculated
800
720
640
560
480
400
320
240
160
80
0
.2
.4
.6
.8
1.0
x_{21}

Carbon Tetrachloride/Benzene

T = 70°C



System: n-Octane/Benzene T= 55°C.

Reference: Elshayl I.M.,Lu B.C.Y.:J.App.Chem.18,277(1968)

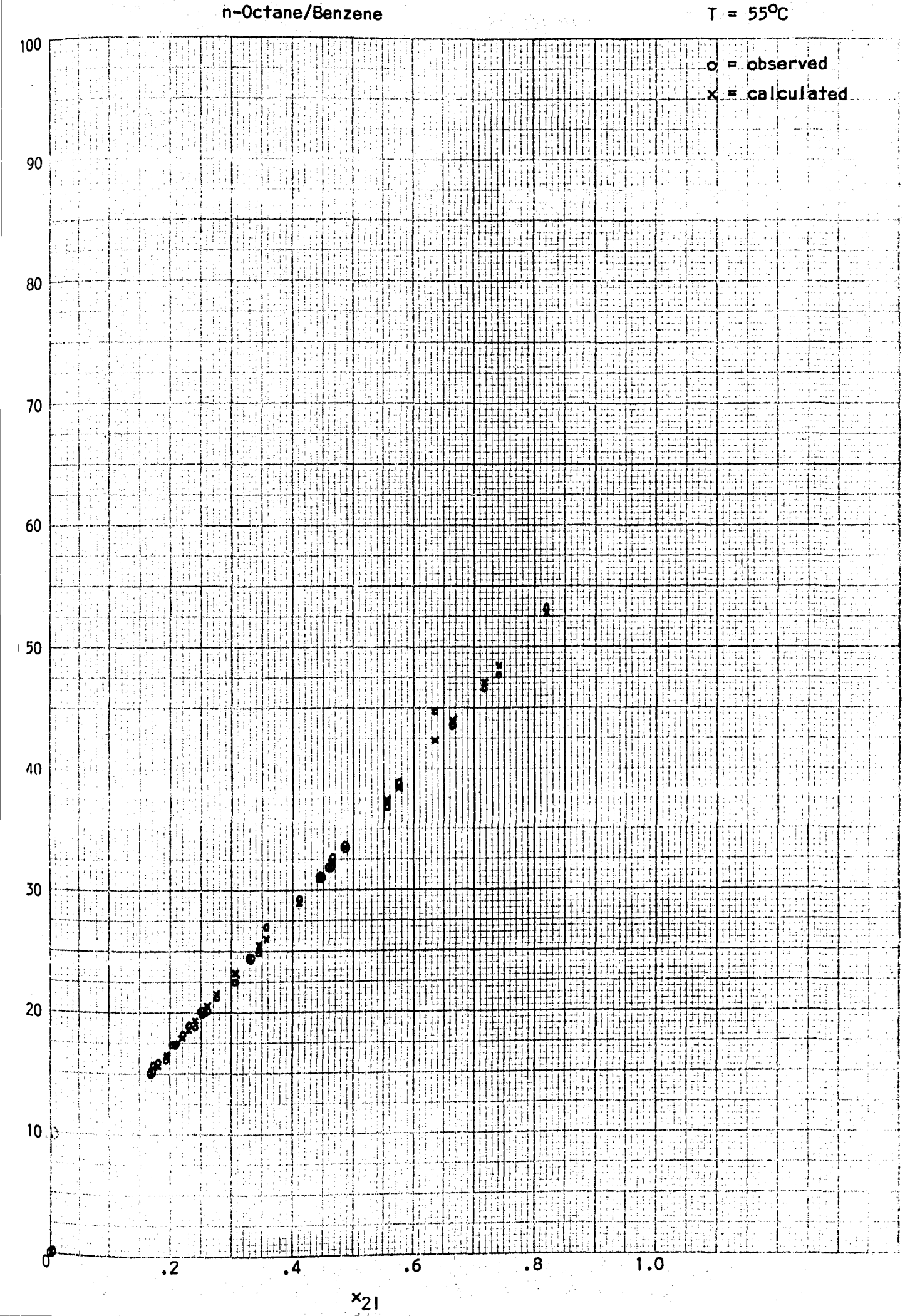
P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
295.40	0.1724	0.0509	15.0359	1.2640	0.9935	0.1046
292.50	0.1725	0.0538	15.7365	1.3221	0.9808	0.1297
290.50	0.1816	0.0560	16.2680	1.2983	0.9826	0.1209
286.70	0.1958	0.0560	16.0552	1.1884	0.9869	0.0807
284.00	0.2070	0.0617	17.5228	1.2268	0.9854	0.0951
283.10	0.2197	0.0652	18.4581	1.2176	0.9946	0.0878
279.40	0.2300	0.0684	19.1110	1.2042	0.9913	0.0845
276.60	0.2530	0.0720	19.9152	1.1408	1.0077	0.0539
275.50	0.2399	0.0679	18.7065	1.1301	0.9907	0.0571
274.00	0.2611	0.0741	20.3034	1.1270	1.0069	0.0489
267.50	0.2780	0.0801	21.4267	1.1170	0.9995	0.0483
264.80	0.3060	0.0850	22.5080	1.0660	1.0238	0.0175
259.80	0.3279	0.0939	24.3952	1.0782	1.0271	0.0211
252.30	0.3464	0.0987	24.9020	1.0419	1.0203	0.0091
252.10	0.3579	0.1075	27.1007	1.0974	1.0276	0.0285
241.30	0.4109	0.1219	29.4145	1.0375	1.0548	-0.0072
230.40	0.4465	0.1350	31.1040	1.0096	1.0559	-0.0195
227.50	0.4608	0.1406	31.9865	1.0060	1.0633	-0.0241
226.80	0.4664	0.1450	32.8860	1.0219	1.0657	-0.0182
218.70	0.4895	0.1529	33.4392	0.9900	1.0642	-0.0314
205.10	0.5550	0.1791	36.7334	0.9592	1.1095	-0.0632
199.10	0.5740	0.1907	37.9684	0.9587	1.1092	-0.0633
181.20	0.6370	0.2470	44.7564	1.0183	1.1023	-0.0344
171.80	0.6661	0.2530	43.4654	0.9457	1.1271	-0.0762
156.00	0.7189	0.2980	46.4880	0.9372	1.1425	-0.0860
143.40	0.7411	0.3324	47.6662	0.9321	1.0844	-0.0657
126.60	0.8167	0.4217	53.3872	0.9474	1.1713	-0.0921

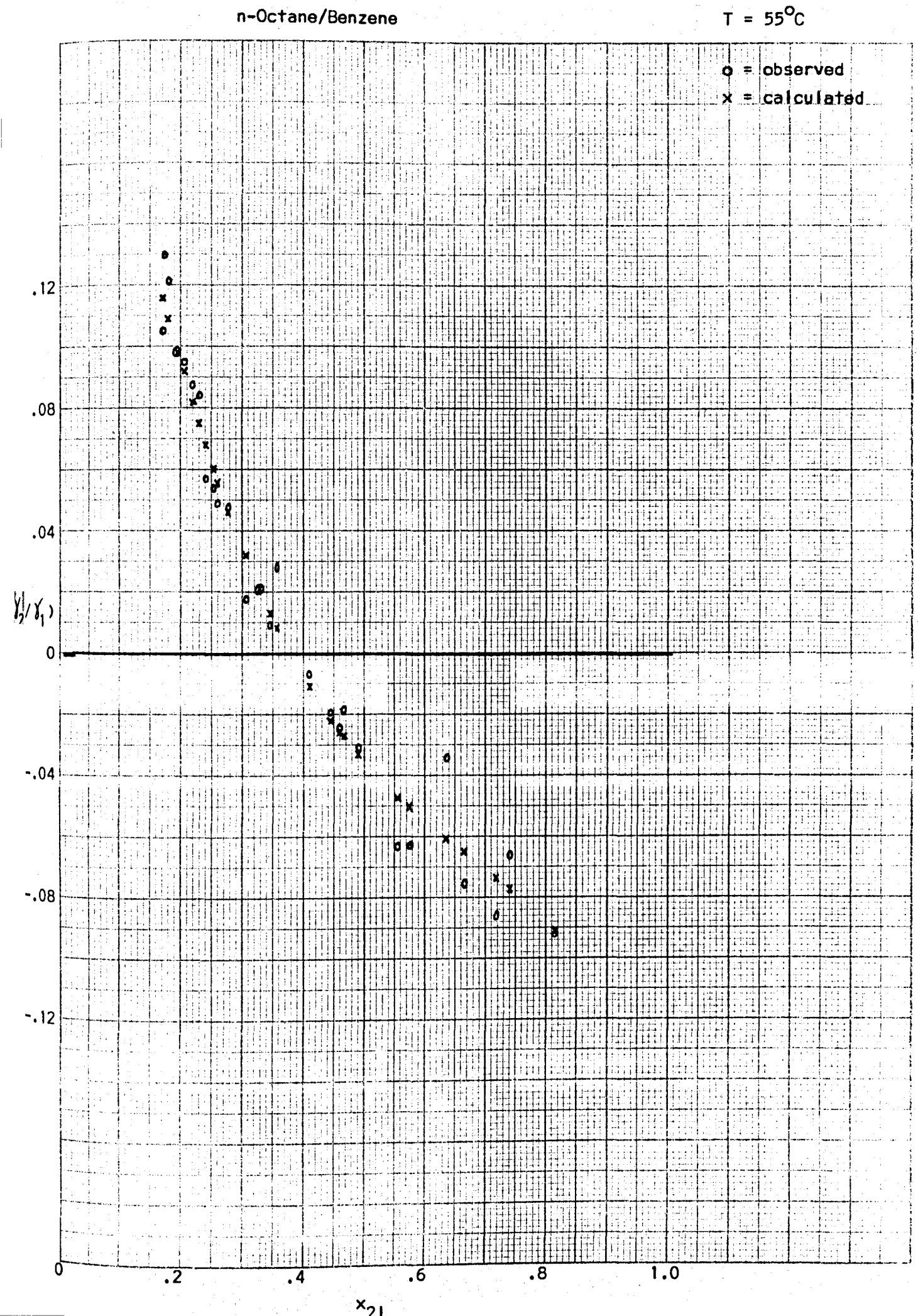
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	111.3437	6.6320	16.7888	15.0123	0.0235
2	-179.6870	44.4284	--4.0444	15.0192	0.7173
3	246.1285	91.0784	2.7024	15.6403	0.6277
4	-117.6120	58.1516	-2.0225	16.5870	-0.5318
				17.3159	0.2069
Degrees of Freedom= 24				18.1251	0.3330
Confidence in First Term= 99.5%+				18.7691	0.3418
Confidence in Last Term= 95.0%+				20.1724	-0.2572
				19.3787	-0.6722
				20.6565	-0.3531
				21.6522	-0.2255
				23.2671	-0.7591
				24.5077	-0.1124
				25.5454	-0.6433
				26.1872	0.9135
				29.1357	0.2788
				31.1268	-0.0228
				31.9237	0.0538
				32.2494	0.6366
				33.5637	-0.1244
				37.3654	-0.6320
				38.4891	-0.5207
				42.2680	2.4884
				44.0289	-0.5635
				47.2121	-0.7241
				48.5322	-0.8660
				52.8394	0.5523

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.2928	0.0345	8.4782	0.1159	-0.0113
1	-1.2939	0.2668	-4.8499	0.1158	0.0139
2	1.6972	0.6107	2.7790	0.1088	0.0122
3	-0.8436	0.4255	-1.9828	0.0982	-0.0175
				0.0902	0.0049
Degrees of Freedom= 23				0.0815	0.0063
Integral at x=1: 0.0007				0.0747	0.0098
Error in Integral: 0.0113				0.0604	-0.0065
				0.0684	-0.0113
				0.0557	-0.0067
				0.0461	0.0021
				0.0316	-0.0141
				0.0213	-0.0002
				0.0132	-0.0041
				0.0084	0.0201
				-0.0108	0.0037
				-0.0217	0.0022
				-0.0256	0.0015
				-0.0271	0.0088
				-0.0328	0.0015
				-0.0468	-0.0165
				-0.0503	-0.0131
				-0.0608	0.0264
				-0.0654	-0.0108
				-0.0737	-0.0123
				-0.0773	0.0117
				-0.0915	-0.0007


n-Octane/Benzene
T = 55°C
o = observed
x = calculated
100
90
80
70
60
50
40
30
20
10
0
.2
.4
.6
.8
1.0
x_{21}


n-Octane/Benzene
T = 55°C
o = observed
x = calculated
.12
.08
.04
0
-.04
-.08
-.12
γ_2'/γ_1
0
.2
.4
.6
.8
1.0
x_{21}

System: n-Octane/Benzene T= 65°C.

Reference: Elshayl I.M.,Lu B.C.Y.:J. App.Chem.18,277(1968)

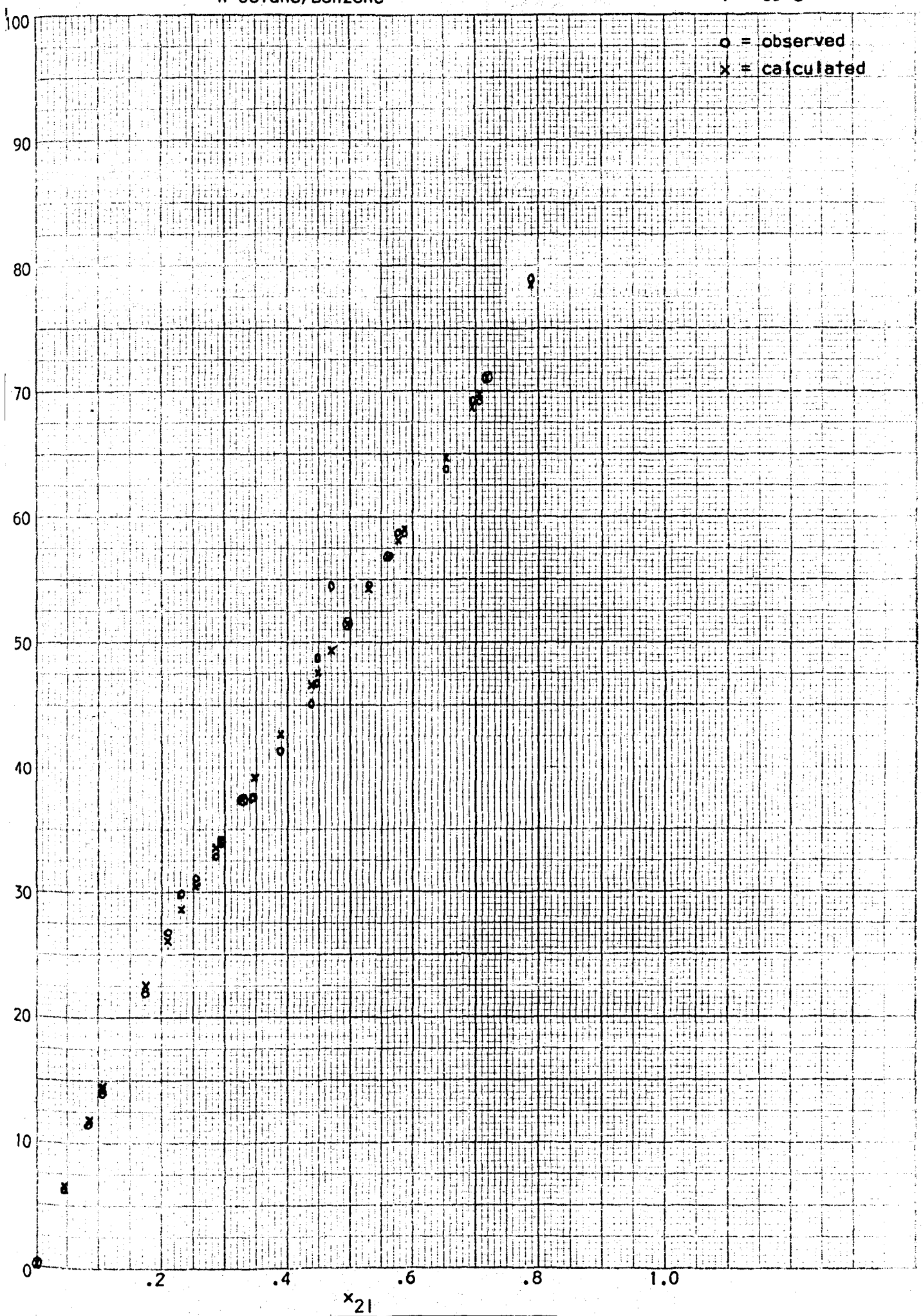
P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1 *	$\log(\gamma_2/\gamma_1)$
450.50	0.0459	0.0141	6.3520	1.4121	1.0098	0.1456
440.10	0.0848	0.0259	11.3986	1.3716	1.0161	0.1303
434.60	0.1060	0.0321	13.9507	1.3430	1.0207	0.1192
414.50	0.1750	0.0530	21.9685	1.2810	1.0321	0.0938
409.90	0.2110	0.0657	26.9304	1.3024	1.0529	0.0923
397.20	0.2337	0.0752	29.8694	1.3042	1.0398	0.0984
396.80	0.2528	0.0786	31.1885	1.2589	1.0614	0.0741
383.90	0.2850	0.0858	32.9386	1.1793	1.0648	0.0444
380.30	0.2915	0.0892	33.9228	1.1875	1.0605	0.0491
368.90	0.3270	0.1010	37.2589	1.1627	1.0689	0.0365
361.80	0.3481	0.1040	37.6272	1.1030	1.0787	0.0097
348.60	0.3888	0.1188	41.4137	1.0869	1.0902	-0.0013
337.00	0.4370	0.1340	45.1580	1.0545	1.1244	-0.0279
336.50	0.4480	0.1450	48.7925	1.1113	1.1306	-0.0075
329.10	0.4450	0.1420	46.7322	1.0716	1.1036	-0.0128
321.70	0.4699	0.1700	54.6890	1.1876	1.0926	0.0362
311.60	0.4958	0.1647	51.3205	1.0562	1.1198	-0.0254
301.00	0.5297	0.1813	54.5713	1.0513	1.1366	-0.0339
289.00	0.5600	0.1970	56.9330	1.0374	1.1441	-0.0425
282.70	0.5769	0.2009	56.7944	1.0046	1.1582	-0.0618
277.40	0.5860	0.2119	58.7811	1.0236	1.1455	-0.0489
251.60	0.6520	0.2534	63.7554	0.9978	1.1709	-0.0695
230.90	0.6938	0.2985	68.9236	1.0137	1.1475	-0.0538
227.90	0.7049	0.3040	69.2816	1.0029	1.1660	-0.0654
223.30	0.7180	0.3184	71.0987	1.0104	1.1708	-0.0639
193.50	0.7890	0.4090	79.1415	1.0235	1.1757	-0.0602

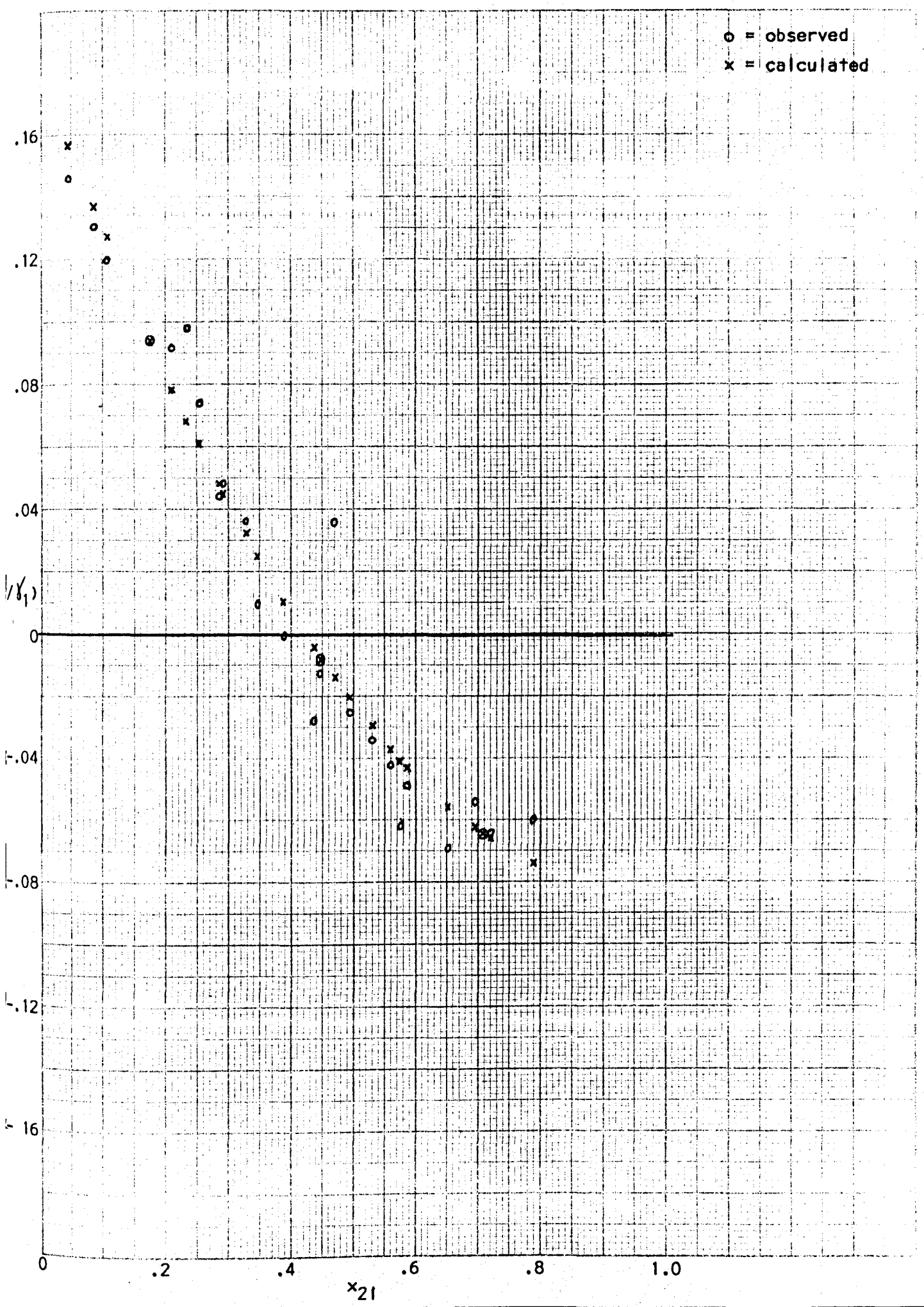
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	150.5511	5.9050	25.4955	6.6170	-0.2649
2	-143.8301	22.8716	-6.2886	11.7936	-0.3950
3	100.2642	21.1887	4.7320	14.4618	-0.5111
				22.4790	-0.5105
Degrees of Freedom= 24				26.3047	0.6257
Confidence in First Term= 99.5%+				28.6082	1.2613
Confidence in Last Term= 99.5%+				30.4873	0.7012
				33.5455	-0.6069
				34.1476	-0.2248
				37.3564	-0.0975
				39.2076	-1.5804
				42.6850	-1.2713
				46.6912	-1.5332
				47.5949	1.1976
				47.3487	-0.6165
				49.3885	5.3005
				51.5071	-0.1866
				54.2925	0.2788
				56.8115	0.1215
				58.2351	-1.4407
				59.0085	-0.2274
				64.8066	-1.0512
				68.7034	0.2202
				69.7745	-0.4929
				71.0603	0.0385
				78.4943	0.6472

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1820	0.0120	15.1301	0.1572	-0.0116
1	-0.5535	0.0636	-8.7005	0.1372	-0.0069
2	0.2899	0.0745	3.8900	0.1266	-0.0074
				0.0940	-0.0002
Degrees of Freedom= 23				0.0781	0.0142
Integral at x=1: 0.0019				0.0685	0.0299-
Error in Integral: 0.0149				0.0606	0.0135
				0.0478	-0.0034
				0.0453	0.0038
				0.0320	0.0045
				0.0245	-0.0148
				0.0106	-0.0119
				-0.0045	-0.0234
				-0.0078	0.0003
				-0.0069	-0.0059
				-0.0141	0.0503
				-0.0212	-0.0042
				-0.0299	-0.0040
				-0.0371	-0.0054
				-0.0408	-0.0209
				-0.0428	-0.0061
				-0.0557	-0.0138
				-0.0625	0.0087
				-0.0641	-0.0013
				-0.0660	0.0020
				-0.0743	0.0141


n-Octane/Benzene
T = 65°C
o = observed
x = calculated
100
90
80
70
60
50
40
30
20
10
0
.2
.4
.6
.8
1.0
x21


n-Octane/Benzene
T = 65°C
o = observed
x = calculated
.16
.12
.08
.04
0
-.04
-.08
-.12
-.16
$\ln(\gamma_1)$
0
.2
.4
.6
.8
1.0
x_{21}

System: n-Octane/Benzene T= 75°C.

Reference: Elshayl I.M.,Lu B.C.Y.:J.App.Chem.18,277(1968)

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
628.40	0.0430	0.0150	9.4260	1.5223	1.0075	0.1792
595.60	0.1180	0.0410	24.4196	1.4371	1.0087	0.1537
544.90	0.2650	0.0870	47.4063	1.2423	1.0543	0.0712
530.90	0.2790	0.0909	48.2588	1.2012	1.0427	0.0614
502.70	0.3495	0.1450	72.8915	1.4483	1.0292	0.1483
485.20	0.3909	0.1320	64.0464	1.1378	1.0770	0.0238
466.90	0.4310	0.1460	68.1674	1.0983	1.0915	0.0027
419.50	0.5270	0.1970	82.6415	1.0890	1.1093	-0.0080
412.70	0.5488	0.2099	86.6257	1.0962	1.1257	-0.0115
399.80	0.5670	0.2178	87.0764	1.0665	1.1250	-0.0232
361.90	0.6350	0.2695	97.5320	1.0666	1.1282	-0.0244
333.80	0.6850	0.3030	101.1414	1.0254	1.1505	-0.0500
277.40	0.7949	0.4290	119.0046	1.0397	1.2029	-0.0633

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	194.7392	10.1200	19.2430
2	-63.6390	16.5171	-3.8529

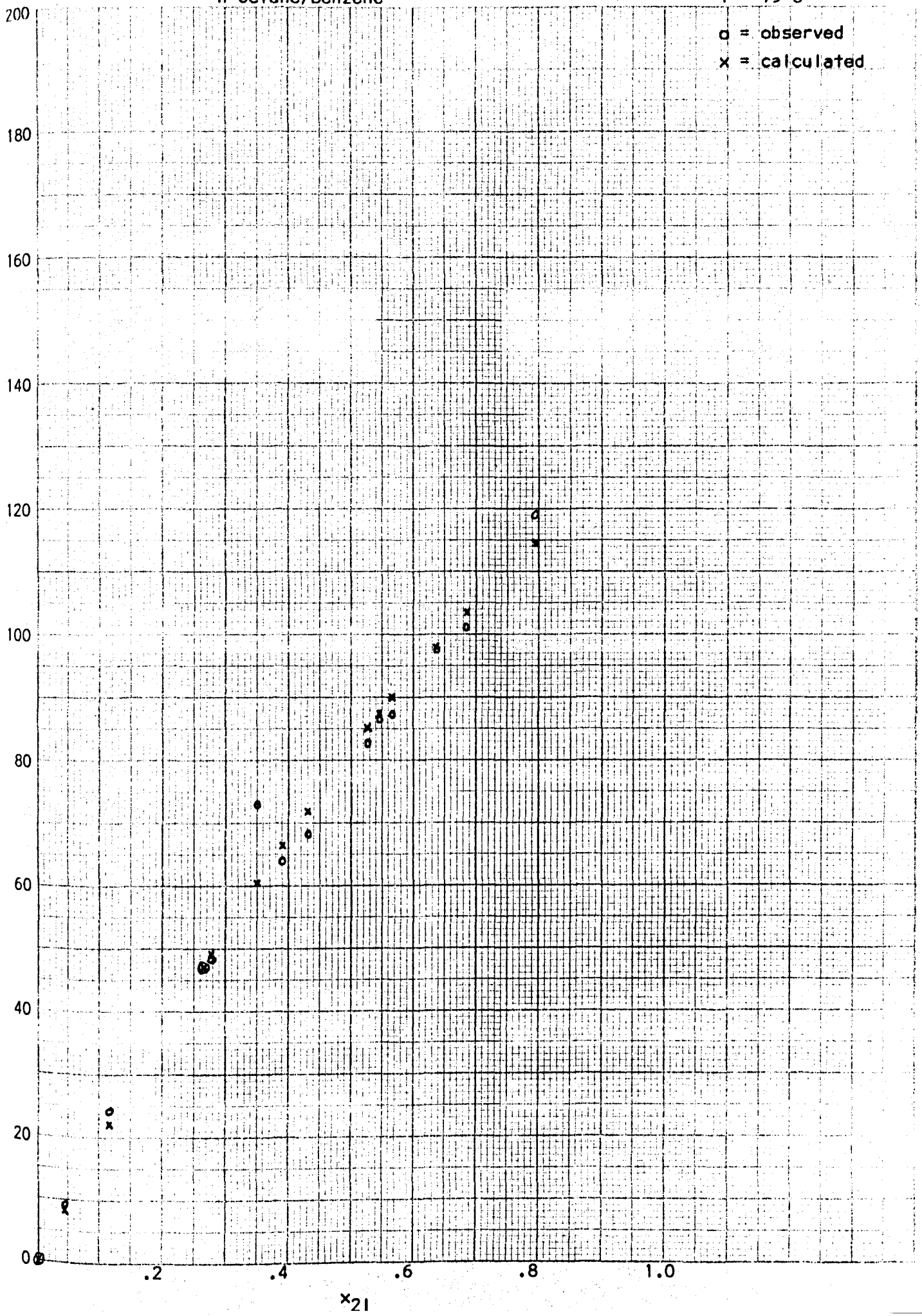
Degrees of Freedom= 12
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%

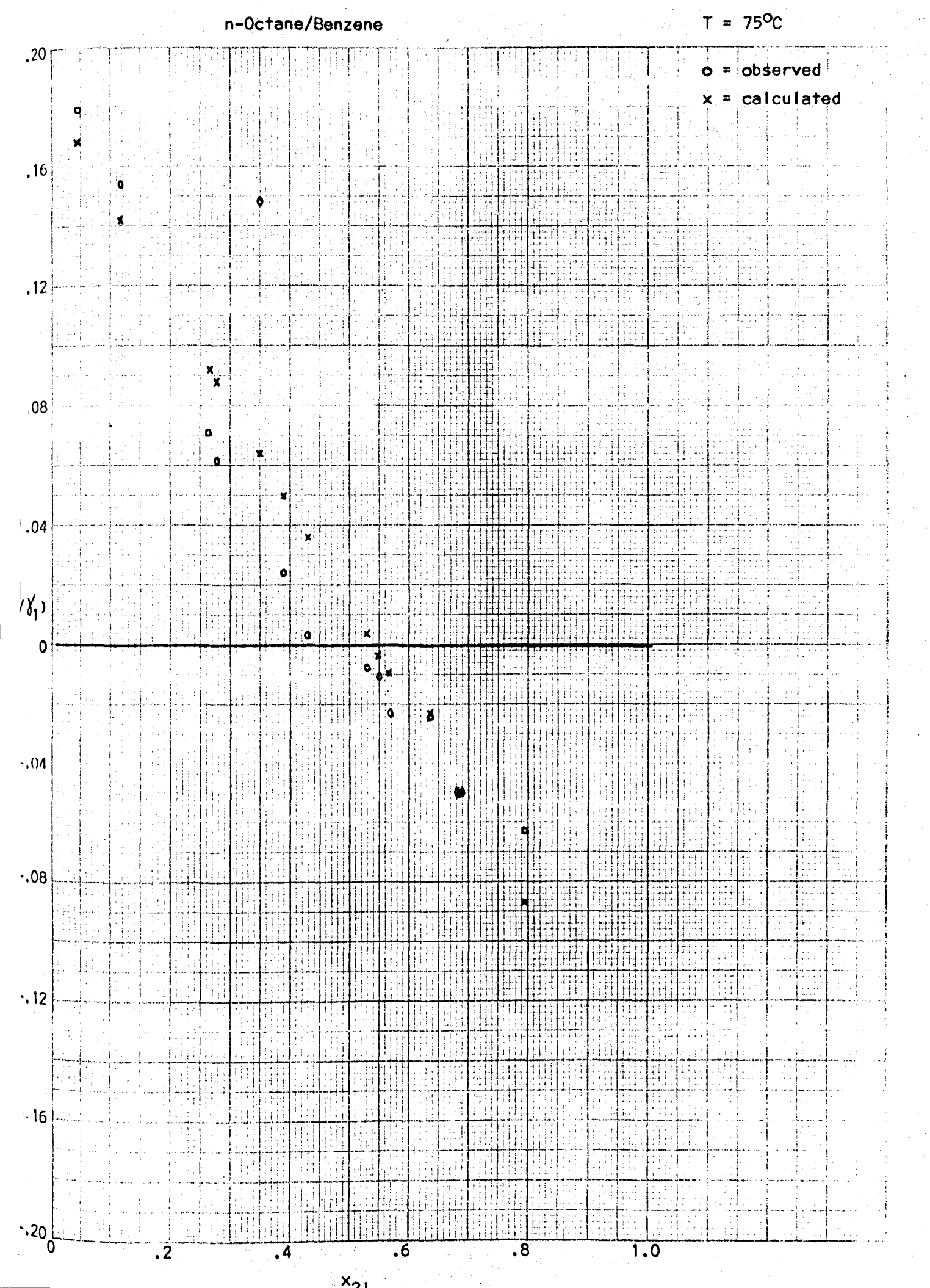
P_2 CALC.	DIF.
8.2561	1.1699
22.0931	2.3265
47.1368	0.2695
49.3785	-1.1297
60.2878	12.6037
66.3993	-2.3529
72.1110	-3.9436
84.9532	-2.3117
87.7060	-1.0803
89.9579	-2.8815
97.9986	-0.4665
103.5354	-2.3940
114.5869	4.4177

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1822	0.0202	9.0020	0.1676	0.0116
1	-0.3387	0.0419	-8.0787	0.1422	0.0115
				0.0924	-0.0212
				0.0877	-0.0262
				0.0638	0.0845
				0.0498	-0.0259
				0.0362	-0.0335
				0.0037	-0.0117
				-0.0037	-0.0078
				-0.0099	-0.0133
				-0.0329	0.0085
				-0.0498	-0.0002
				-0.0870	0.0237

Degrees of Freedom= 11
Integral at x=1: 0.0128
Error in Integral: 0.0283


n-Octane/Benzene
T = 75°C
o = observed
x = calculated
200
180
160
140
120
100
80
60
40
20
0
.2
.4
.6
.8
1.0
x21


n-Octane/Benzene
T = 75°C
o = observed
x = calculated
.20
.16
.12
.08
.04
0
-.04
-.08
-.12
-.16
-.20
0
.2
.4
.6
.8
1.0
x_{21}

System: Methane/Benzene 40°C.

Reference; Savvina,Velikovskii(1956:Physico-Chemical Constants of Binary Systems;Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
88.36	0.0100	0.9600	84.8250	1.1765	0.0893	1.1198
353.44	0.0500	0.9900	349.9030	0.9706	0.0930	1.0183
1060.31	0.1300	0.9950	1055.0107	1.1256	0.1523	0.8684
1767.19	0.2300	0.9950	1758.3511	1.0603	0.2869	0.5676
2650.78	0.3100	0.9950	2637.5266	1.1800	0.4802	0.3904
3534.37	0.3800	0.9900	3499.0303	1.2771	1.4252	-0.0476
4417.97	0.4400	0.9800	4329.6082	1.3648	3.9446	-0.4609
5301.56	0.4900	0.9600	5089.4986	1.4406	10.3952	-0.8581
6008.44	0.5500	0.9200	5527.7610	1.3940	26.7042	-1.2821
6750.65	0.7600	0.7600	5130.4974	0.9363	168.7664	-2.2555

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	6627.5103	520.4247	12.7348
2	6818.2659	1136.9479	5.9970

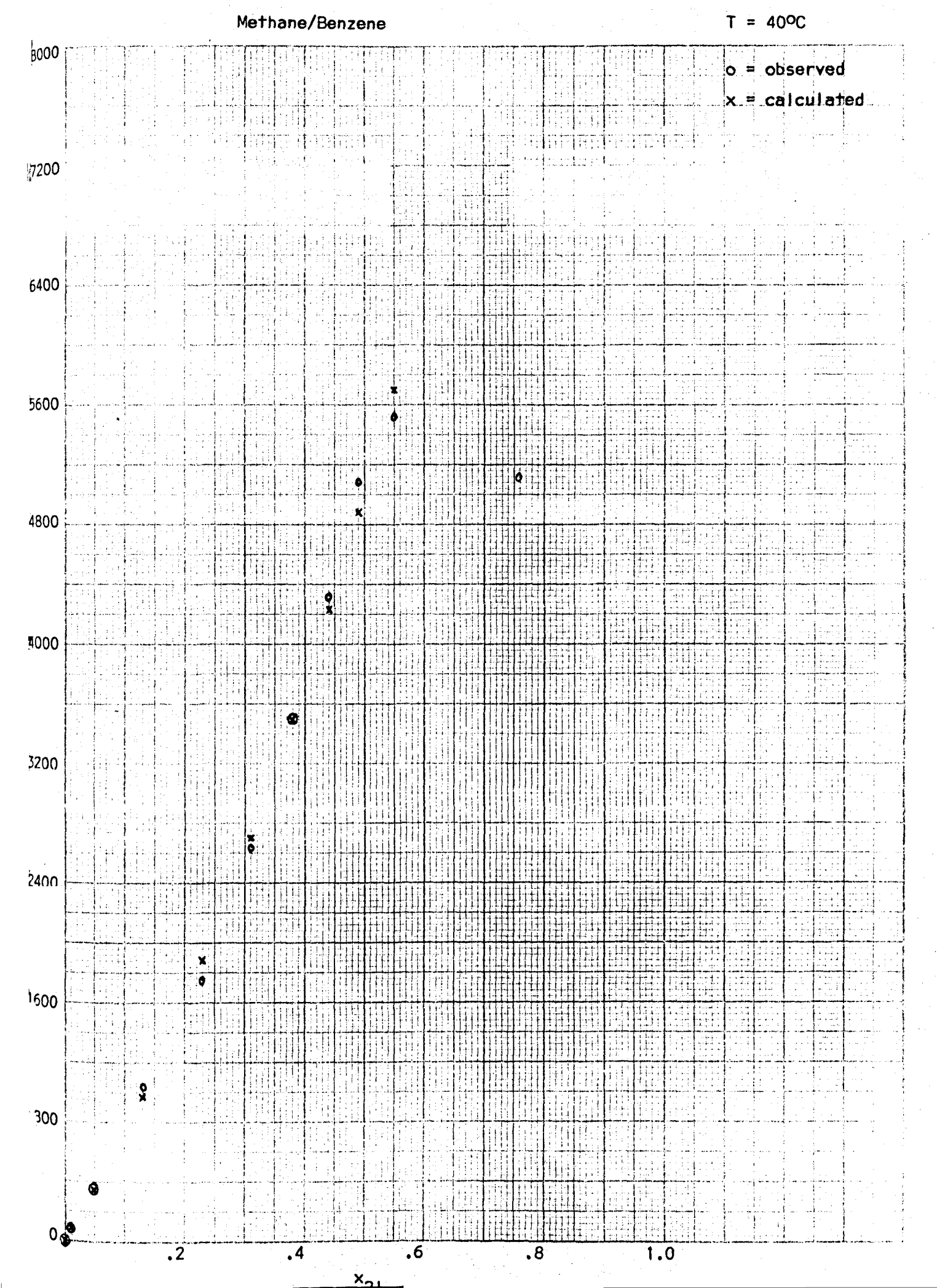
Degrees of Freedom= 8
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

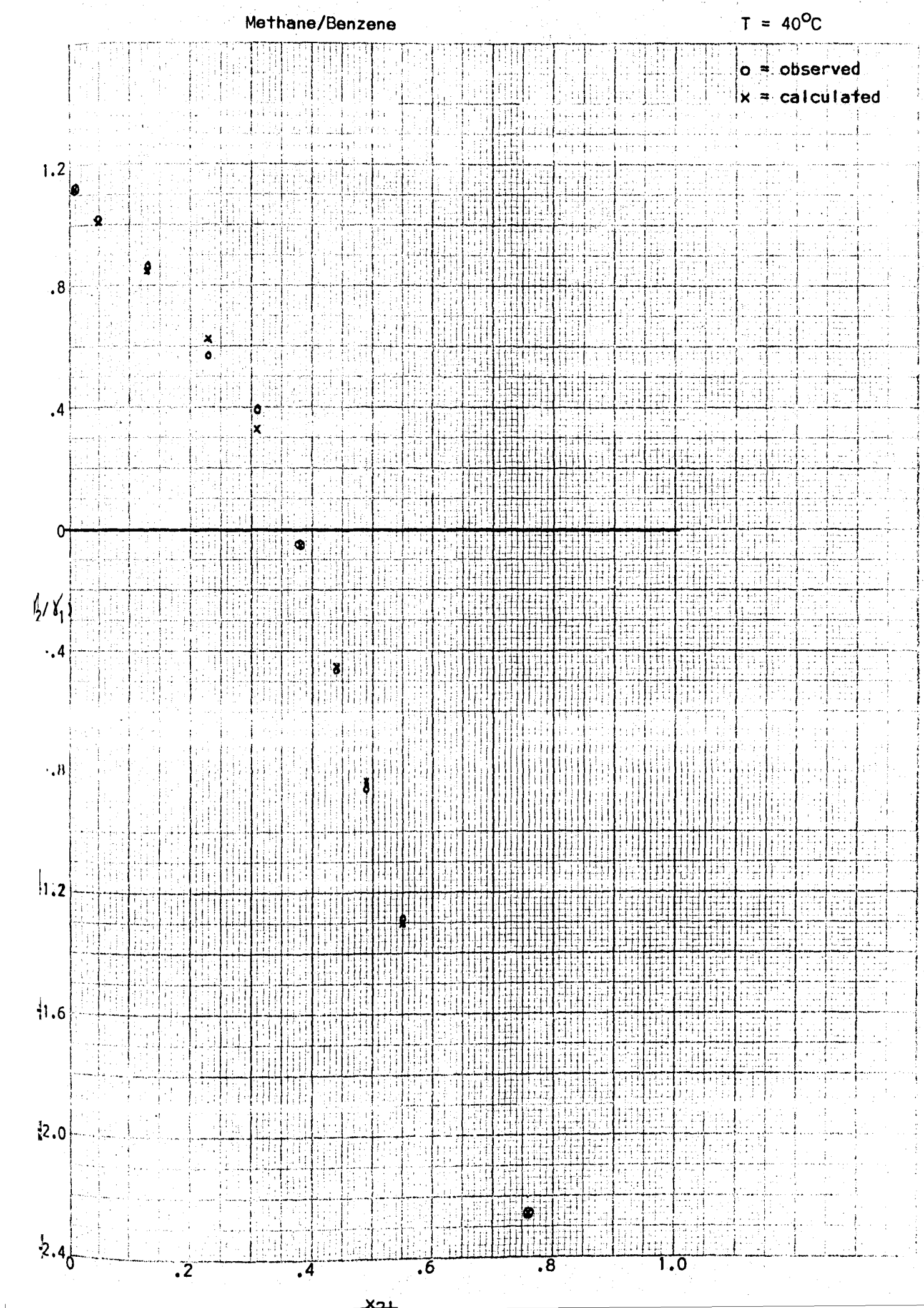
p_2 CALC.	DIF.
66.9569	17.8680
348.4212	1.4819
976.8050	78.2056
1885.0136	-126.6625
2709.7635	-72.2369
3503.0115	-3.9812
4236.1208	93.4874
4884.5457	204.9530
5707.6561	-179.8950

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.1634	0.0457	25.4450	1.1269	-0.0071
1	-3.8262	1.0968	-3.4885	1.0101	0.0082
2	18.1822	6.5462	2.7775	0.8513	0.0171
3	-61.7667	13.6309	-4.5314	0.6287	-0.0611
4	48.2637	9.0159	5.3532	0.3302	0.0602
				-0.0480	0.0004
				-0.4527	-0.0082
				-0.8304	-0.0277
				-1.3009	0.0189
				-2.2548	-0.0007

Degrees of Freedom= 5
Integral at x=1: -0.4780
Error in Integral: 0.0299


Methane/Benzene
T = 40°C
o = observed
x = calculated
8000
7200
6400
5600
4800
4000
3200
2400
1600
300
0
.2
.4
.6
.8
1.0
x_{21}


Methane/Benzene
T = 40°C
o = observed
x = calculated
1.2
.8
.4
0
$\ln(\gamma_2/\gamma_1)$
-.4
-.8
-1.2
-1.6
-2.0
-2.4
0
.2
.4
.6
.8
1.0
x_{21}

System: Methane/Benzene T= 60°C.

Reference: Savvina,Velikovskii(1956):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
88.36	0.0050	0.9500	83.9414	2.3898	0.0740	1.5088
353.44	0.0450	0.9800	346.3687	1.0957	0.1234	0.9483
1060.31	0.1250	0.9900	1049.7091	1.1954	0.2020	0.7721
1767.19	0.2250	0.9900	1749.5152	1.1069	0.3800	0.4642
2650.78	0.3050	0.9900	2624.2727	1.2248	0.6357	0.2848
3534.37	0.3750	0.9800	3463.6866	1.3148	1.8850	-0.1564
4417.97	0.4450	0.9700	4285.4285	1.3708	3.9802	-0.4628
5301.56	0.4950	0.9500	5036.4830	1.4484	8.7485	-0.7809
6008.44	0.5600	0.9000	5407.5923	1.3746	22.7592	-1.2188
6450.23	0.7400	0.7400	4773.1722	0.9182	107.5039	-2.0681

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	7392.5314	552.7094	13.3751
2	4676.5970	1188.7768	3.9340

Degrees of Freedom= 8
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

P_2 CALC.	DIF.
37.0796	46.8618
342.1340	4.2346
997.1383	52.5708
1900.0723	+150.5571
2689.7625	-65.4898
3429.8457	33.8408
4215.7596	69.6690
4805.1862	231.2968
5606.3984	-198.8061

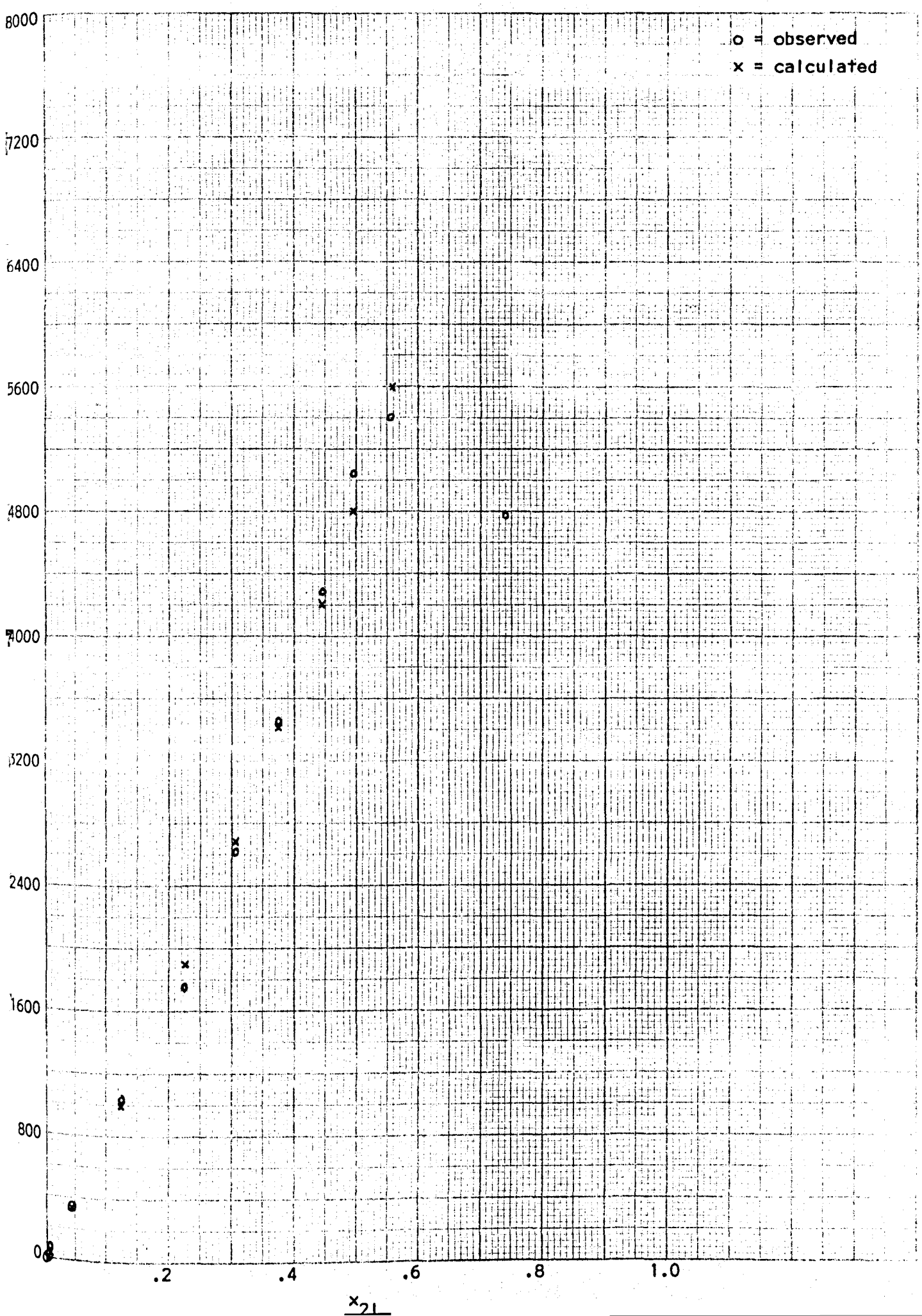
THERMODYNAMIC CONSISTENCY CURVE FITTING:

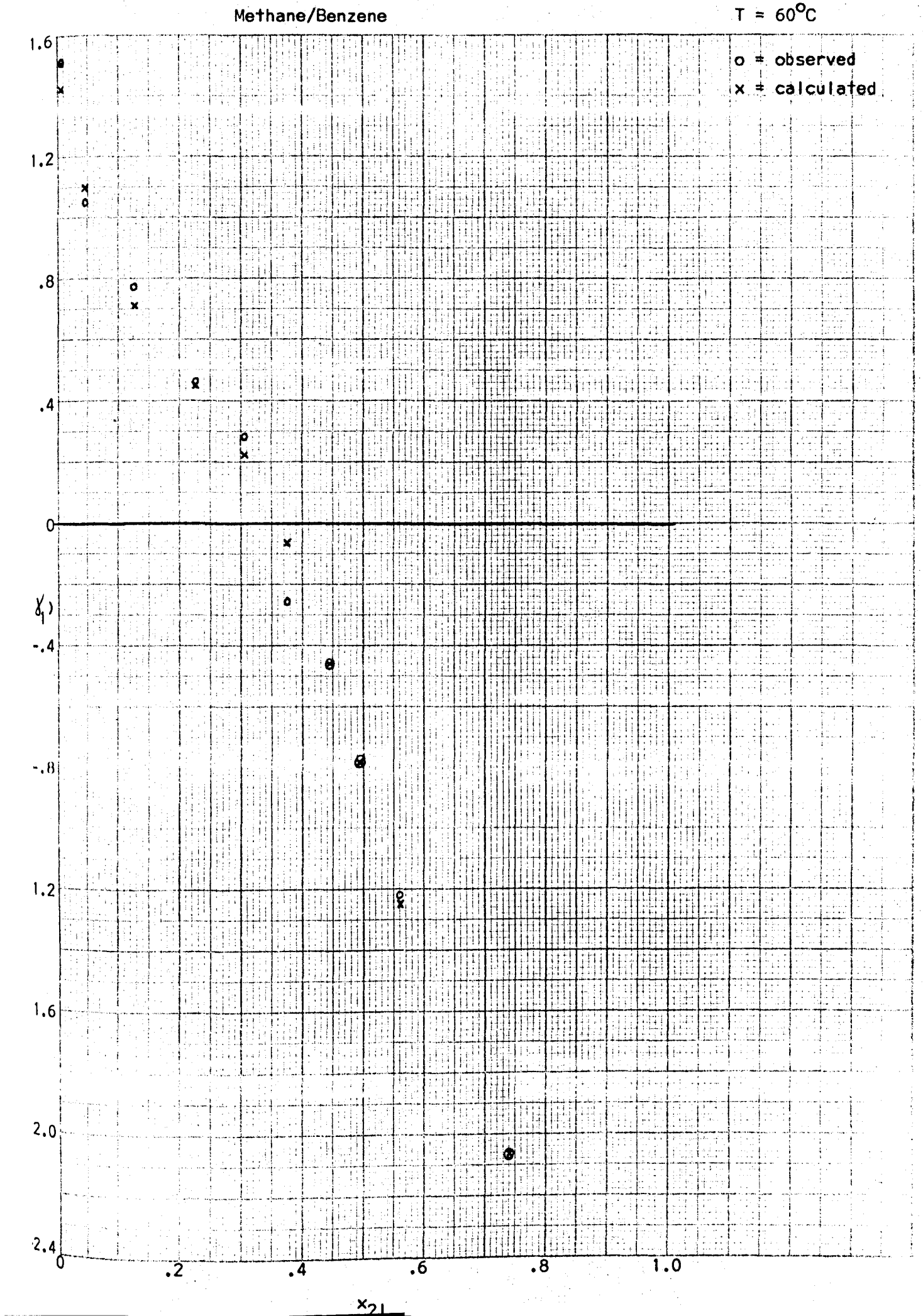
n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.4731	0.0947	15.5506	1.4238	0.0851
1	-10.0839	2.3440	-4.3020	1.0980	-0.1497
2	43.0689	14.3384	3.0037	0.7126	-0.0595
3	-96.7467	30.3787	-3.1847	0.4497	0.0145
4	65.1816	20.4825	3.1823	0.2231	0.0616
				-0.0646	-0.0918
				-0.4549	-0.0079
				-0.7863	0.0054
				-1.2474	0.0287
				-2.0628	-0.0053

Degrees of Freedom= 5
Integral at x=1: -0.3629
Error in Integral: 0.0683

Methane/Benzene

T = 60°C




Methane/Benzene
T = 60°C
o = observed
x = calculated
1.6
1.2
.8
.4
0
-.4
-.8
1.2
1.6
2.0
2.4
0
.2
.4
.6
.8
1.0
x_{21}

System: Methane/Benzene T= 80°C.

Reference: Savvina,Velikovskii(1956):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
176.72	0.0300	0.9300	164.3484	0.8269	0.4251	0.2889
353.44	0.0400	0.9700	342.8343	1.2937	0.3683	0.5457
1060.31	0.1200	0.9800	1039.1060	1.3071	0.8033	0.2114
1767.19	0.2200	0.9800	1731.8433	1.1882	1.5104	-0.1042
2650.78	0.3000	0.9800	2597.7649	1.3071	2.5246	-0.2858
3534.37	0.3700	0.9750	3446.0147	1.4058	4.6751	-0.5218
4417.97	0.4350	0.9500	4197.0692	1.4564	13.0324	-0.9516
5301.56	0.4950	0.9200	4877.4362	1.4873	27.9950	-1.2745
6096.80	0.7100	0.7100	4328.7246	0.9203	203.2265	-2.3436

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	7056.3276	353.8624	19.9409
2	5762.9115	852.2534	6.7620

Degrees of Freedom= 7
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.9%+

P_2 CALC.	DIF.
216.8764	-52.5281
291.4738	51.3605
929.7452	109.3607
1831.3170	-99.4737
2635.5603	-37.7954
3399.7838	46.2309
4159.9894	37.0798
4904.9396	-27.5034
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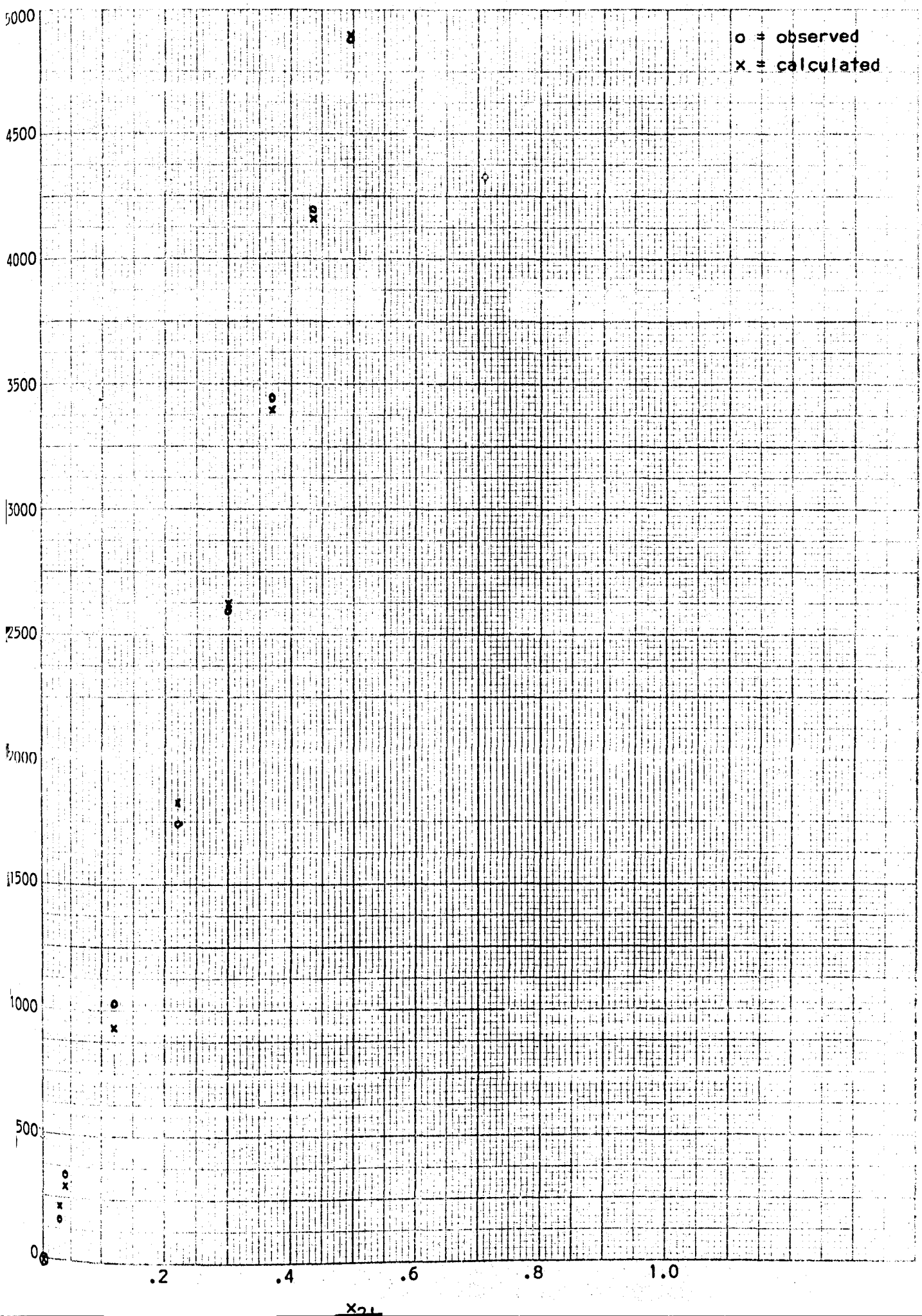
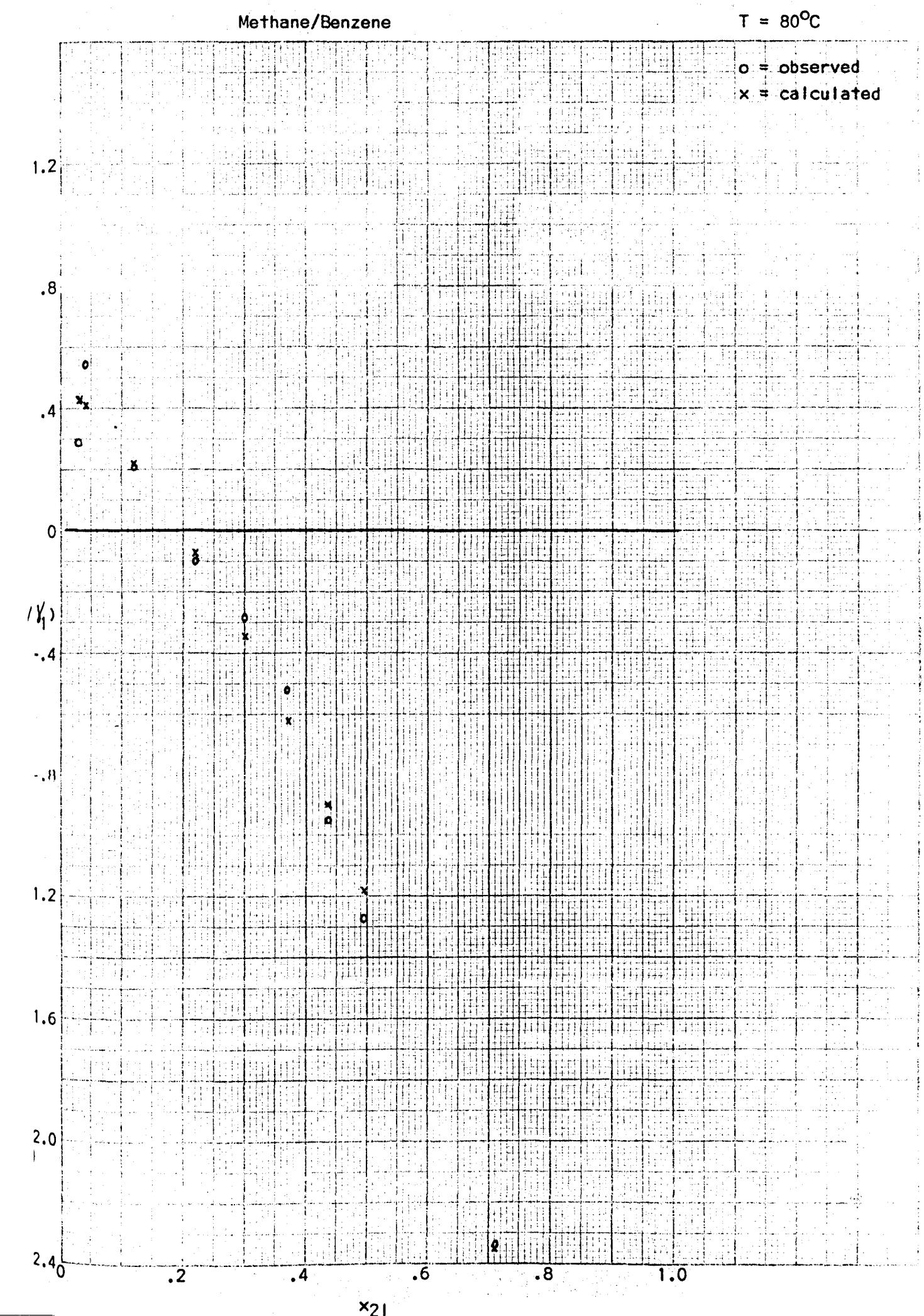
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.4858	0.0797	6.0956	0.4276	-0.1386
1	-1.8494	0.5348	-3.4582	0.4069	0.1388
2	-3.0695	0.7440	-4.1260	0.2197	-0.0083
				-0.0696	-0.0345
				-0.3453	0.0594
				-0.6187	0.0969
				-0.8995	-0.0520
				-1.1818	-0.0927
				-2.3746	0.0310

Degrees of Freedom= 6
Integral at x=1: -1.4621
Error in Integral: 0.0849


Methane/Benzene
T = 80°C
o = observed
× = calculated
5000
4500
4000
3500
3000
2500
2000
1500
1000
500
0
.2
.4
.6
.8
1.0
x21


Methane/Benzene
T = 80°C
o = observed
x = calculated
1.2
.8
.4
0
-.4
-.8
1.2
1.6
2.0
2.4
0
.2
.4
.6
.8
1.0
x_{21}

System: Methane/Benzene T= 100°C.

Reference: Savvina,Velikovskii(1956):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
353.44	0.0350	0.9500	335.7655	1.6096	0.2442	0.8189
1060.31	0.1150	0.9700	1028.5029	1.5006	0.4792	0.4956
1767.19	0.2150	0.9700	1714.1714	1.3377	0.9005	0.1719
2650.78	0.2950	0.9700	2571.2571	1.4624	1.5040	-0.0122
3534.37	0.3650	0.9650	3410.6710	1.5678	2.5974	-0.2192
4417.97	0.4250	0.9400	4152.8895	1.6395	6.1467	-0.5738
5301.56	0.5200	0.8950	4744.8972	1.5310	15.4629	-0.0041
5743.36	0.7200	0.7200	4135.2177	0.9637	76.5781	-1.8998

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	9200.5148	173.5594	53.0108

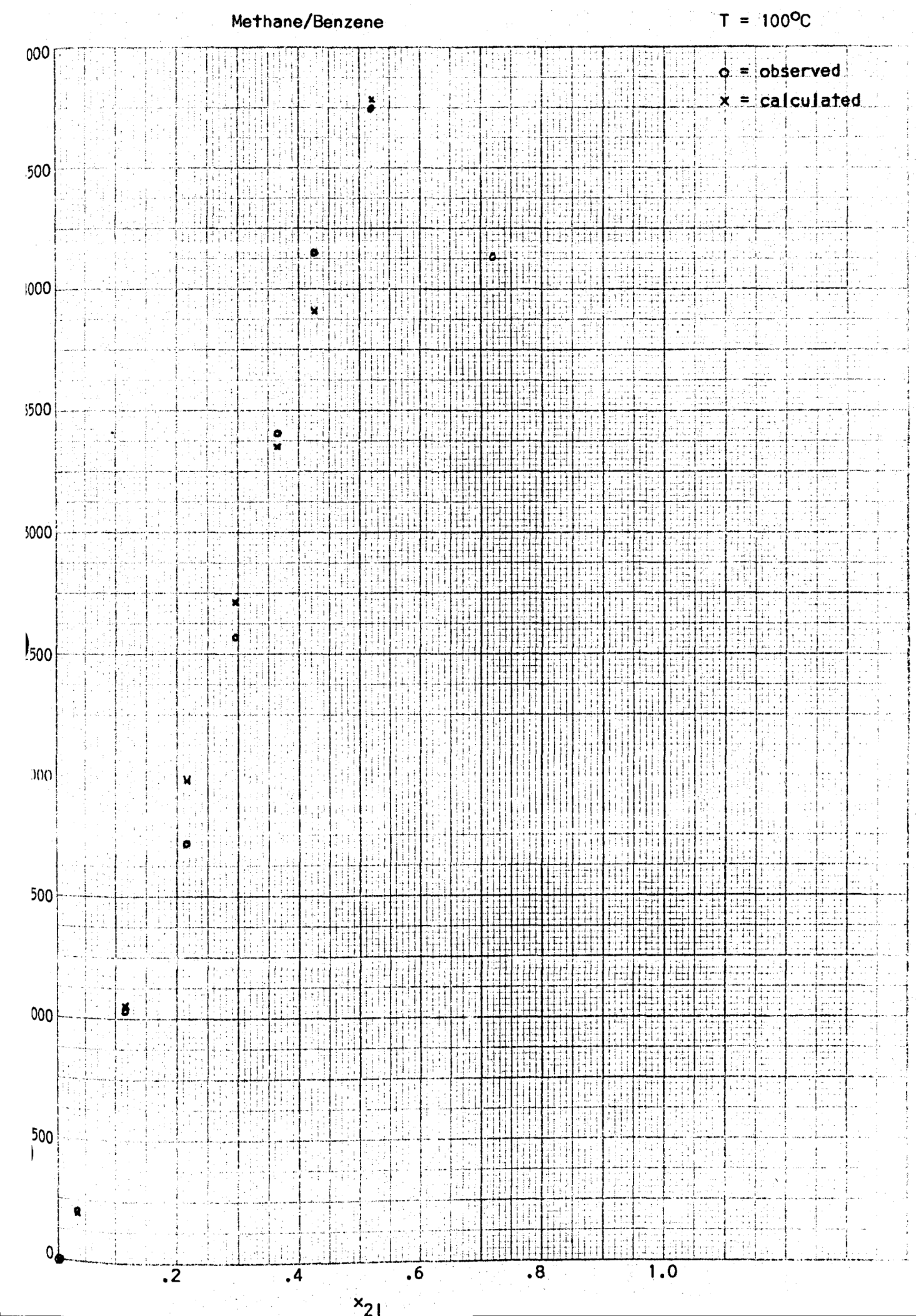
Degrees of Freedom= 7
Confidence in First Term= 99.5%+

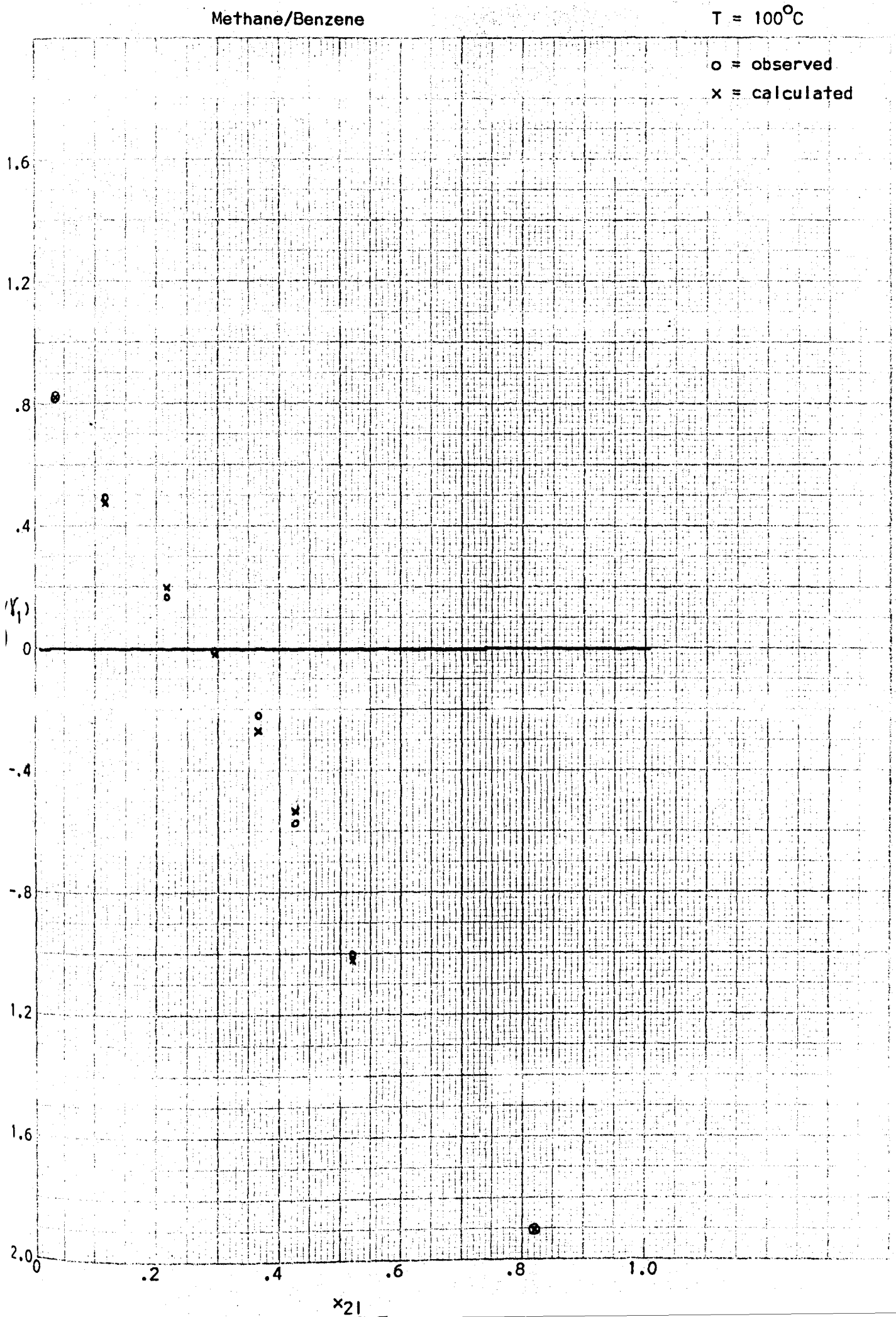
P_2 CALC.	DIF.
322.0180	13.7475
1058.0592	-29.5564
1978.1107	-263.9393
2714.1519	-142.8947
3358.1879	52.4831
3910.2188	242.6707
4784.2677	-39.3705

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.0458	0.0839	12.4662	0.8229	-0.0040
1	-7.2115	1.7581	-4.1018	0.4792	0.0164
2	26.1170	10.1098	2.5833	0.2020	-0.0302
3	-58.9280	21.1734	-2.7831	-0.0200	0.0078
4	39.8262	14.3778	2.7700	-0.2656	0.0464
				-0.5260	-0.0478
				-1.0160	0.0118
				-1.8994	-0.0005

Degrees of Freedom= 3
Integral at x=1: -0.6211
Error in Integral: 0.0270


Methane/Benzene
T = 100°C
o = observed
x = calculated
.2
.4
.6
.8
1.0
x_{21}


Methane/Benzene
T = 100°C
o = observed
x = calculated
1.6
1.2
.8
.4
0
-.4
-.8
1.2
1.6
2.0
0
.2
.4
.6
.8
1.0
x_{21}

System: Methane/Benzene T= 120°C.

Reference: Savvina,Velikovskii(1956):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
353.44	0.0350	0.9200	325.1624	1.6458	0.3256	0.7036
1060.31	0.1100	0.9500	1007.2966	1.6222	0.6619	0.3893
1767.19	0.2100	0.9400	1661.1558	1.4013	1.4913	-0.0270
2650.78	0.2900	0.9400	2491.7337	1.5221	2.4890	-0.2135
3534.37	0.3600	0.9350	3304.6397	1.6261	3.9884	-0.3896
4417.97	0.4200	0.9100	4020.3505	1.6957	7.6172	-0.6523
5301.56	0.5900	0.8000	4241.2489	1.2734	28.7347	-1.3532
5407.59	0.7000	0.7000	3785.3146	0.9579	60.0844	-1.7971

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	10636.0919	1079.7831	9.8502
2	-5228.2259	2281.2517	-2.2998

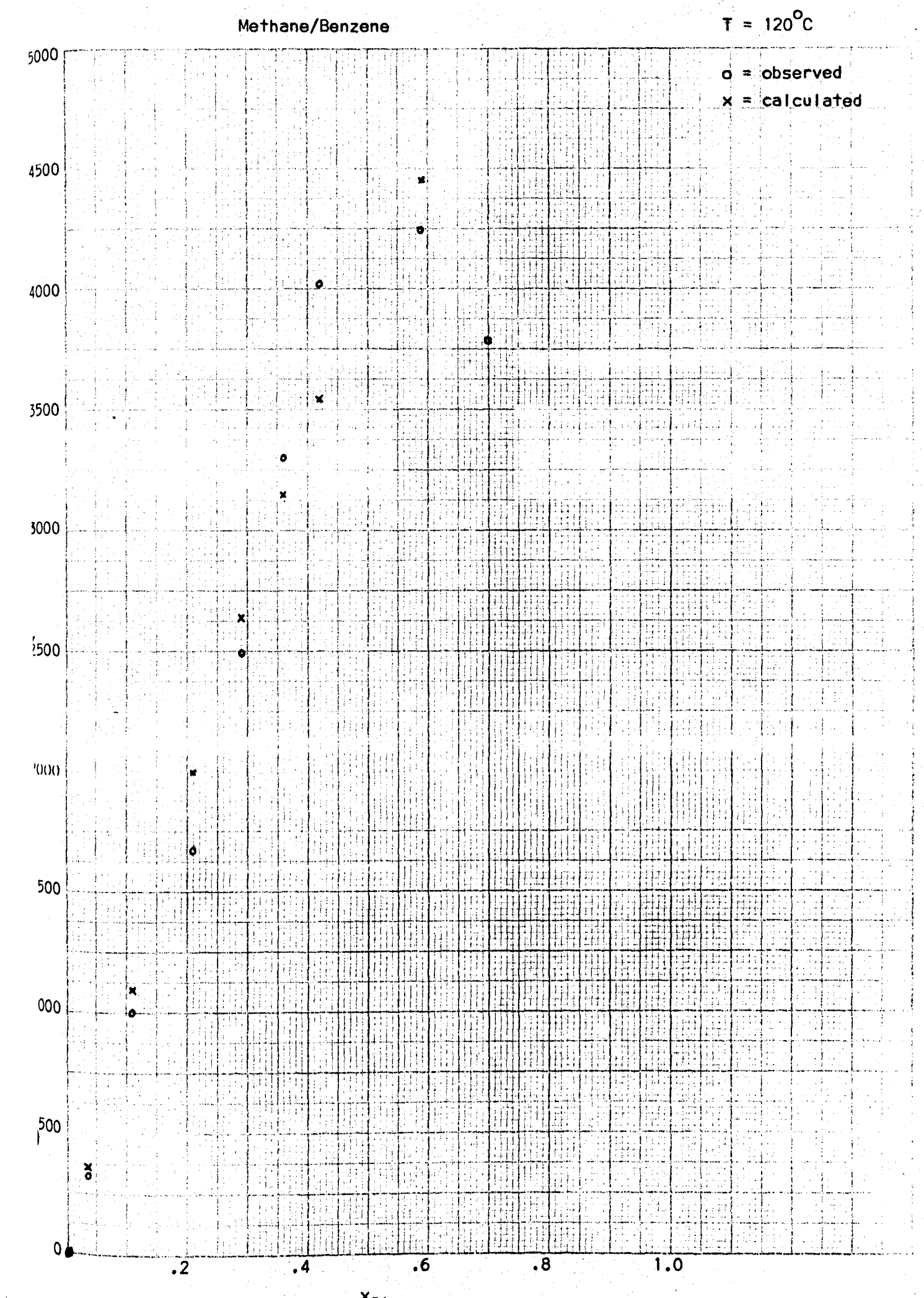
Degrees of Freedom= 6
Confidence in First Term= 99.5%+
Confidence in Last Term= 95.0%+

P_2CALC.	DIF.
365.8586	-40.6962
1106.7086	-99.4120
2003.0145	-341.8587
2644.7728	-153.0391
3151.4150	153.2247
3544.8995	475.4510
4455.3488	-214.0999

THERMODYNAMIC CONSISTENCY CURVE FITTING:

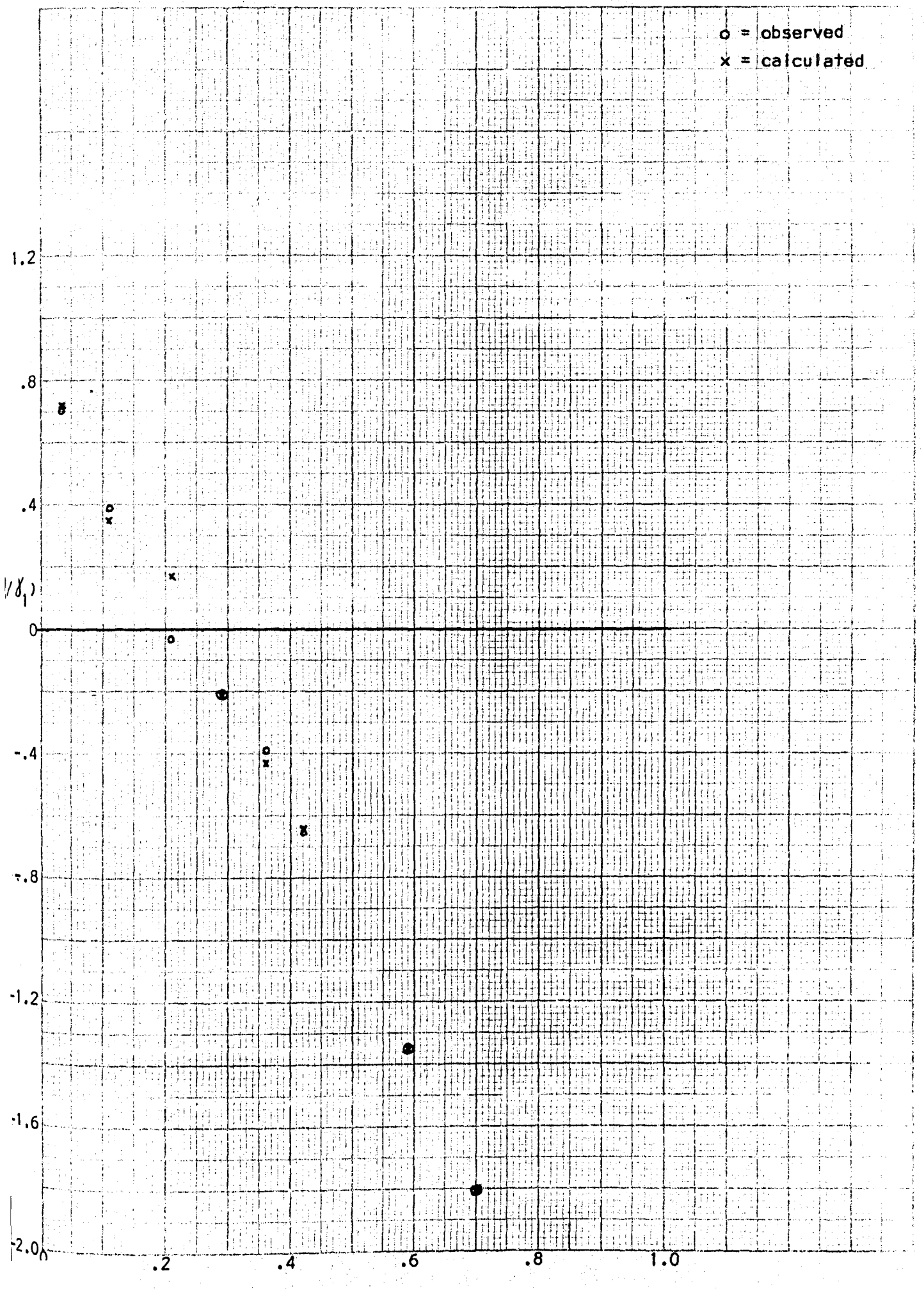
n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.9443	0.0766	12.3299	0.7160	-0.0124
1	-7.1897	1.5361	-4.6806	0.3514	0.0379
2	20.3617	8.5154	2.3912	0.0171	-0.0442
3	-39.0317	17.4532	-2.2364	-0.2123	-0.0012
4	23.7412	11.8491	2.0036	-0.4274	0.0378
				-0.6366	-0.0157
				-1.3492	-0.0040
				-1.7989	0.0018

Degrees of Freedom= 3
Integral at x=1: -0.8730
Error in Integral: 0.0256


Methane/Benzene
T = 120°C
o = observed
× = calculated
5000
4500
4000
3500
3000
2500
000
500
000
500
0
.2
.4
.6
.8
1.0

Methane/Benzene

T = 120°C



System: Methane/Benzene T= 150°C.

Reference: Savvina,Velikovskii(1956):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
353.44	0.0300	0.8800	311.0249	1.9524	0.2301	0.9284
1060.31	0.1050	0.9200	975.4872	1.7496	0.4988	0.5449
1767.19	0.2050	0.9200	1625.8121	1.4936	0.9359	0.2029
2650.78	0.2850	0.9100	2412.2103	1.5940	1.7561	-0.0421
3534.37	0.3550	0.9050	3198.6085	1.6968	2.7398	-0.2080
4417.97	0.4600	0.8400	3711.0928	1.5193	6.8896	-0.6564
4736.06	0.6500	0.6500	3078.4398	0.8919	24.9266	-1.4461

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	8407.6502	180.1639	46.6667

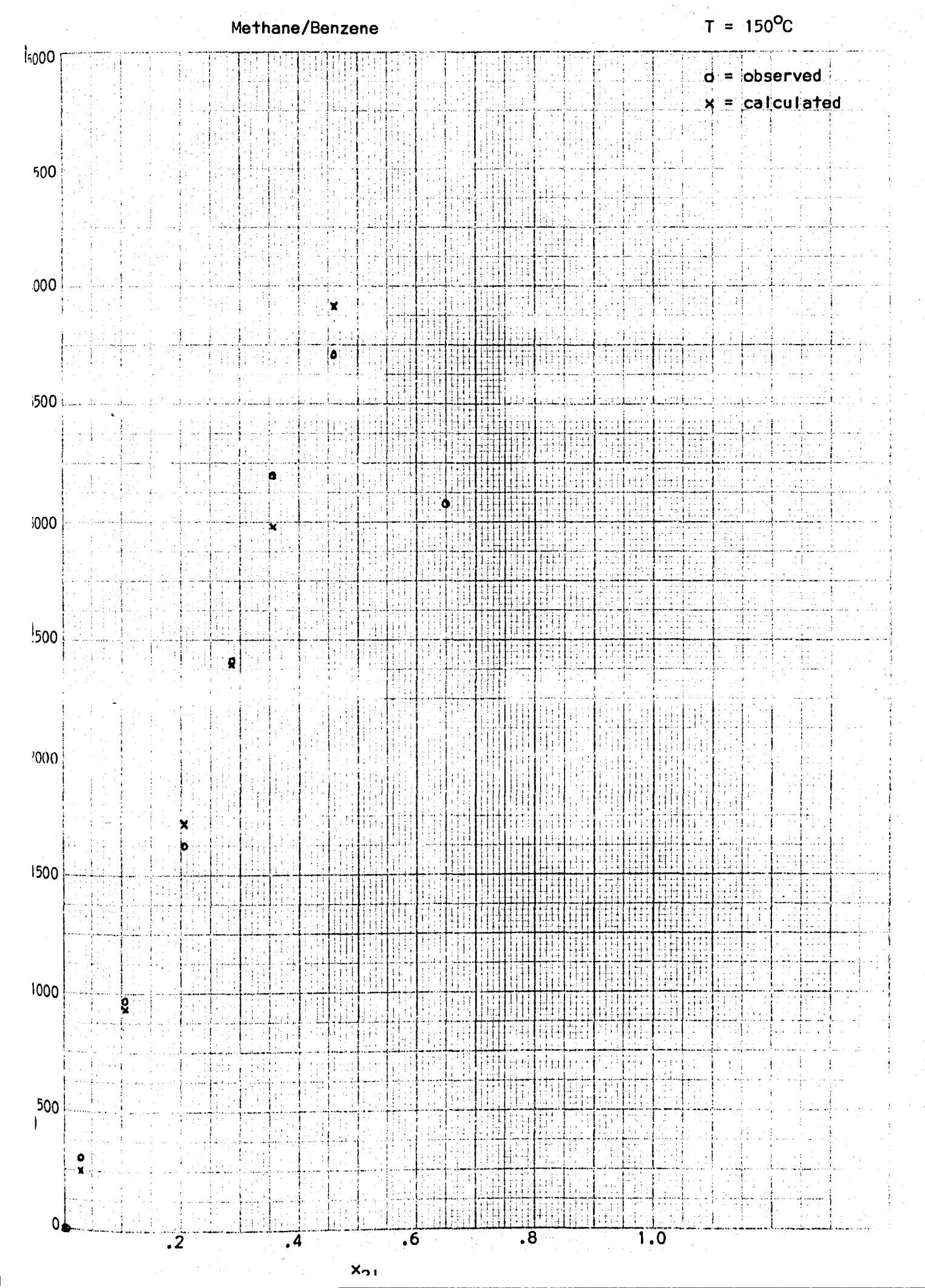
Degrees of Freedom= 6
Confidence in First Term= 99.5%+

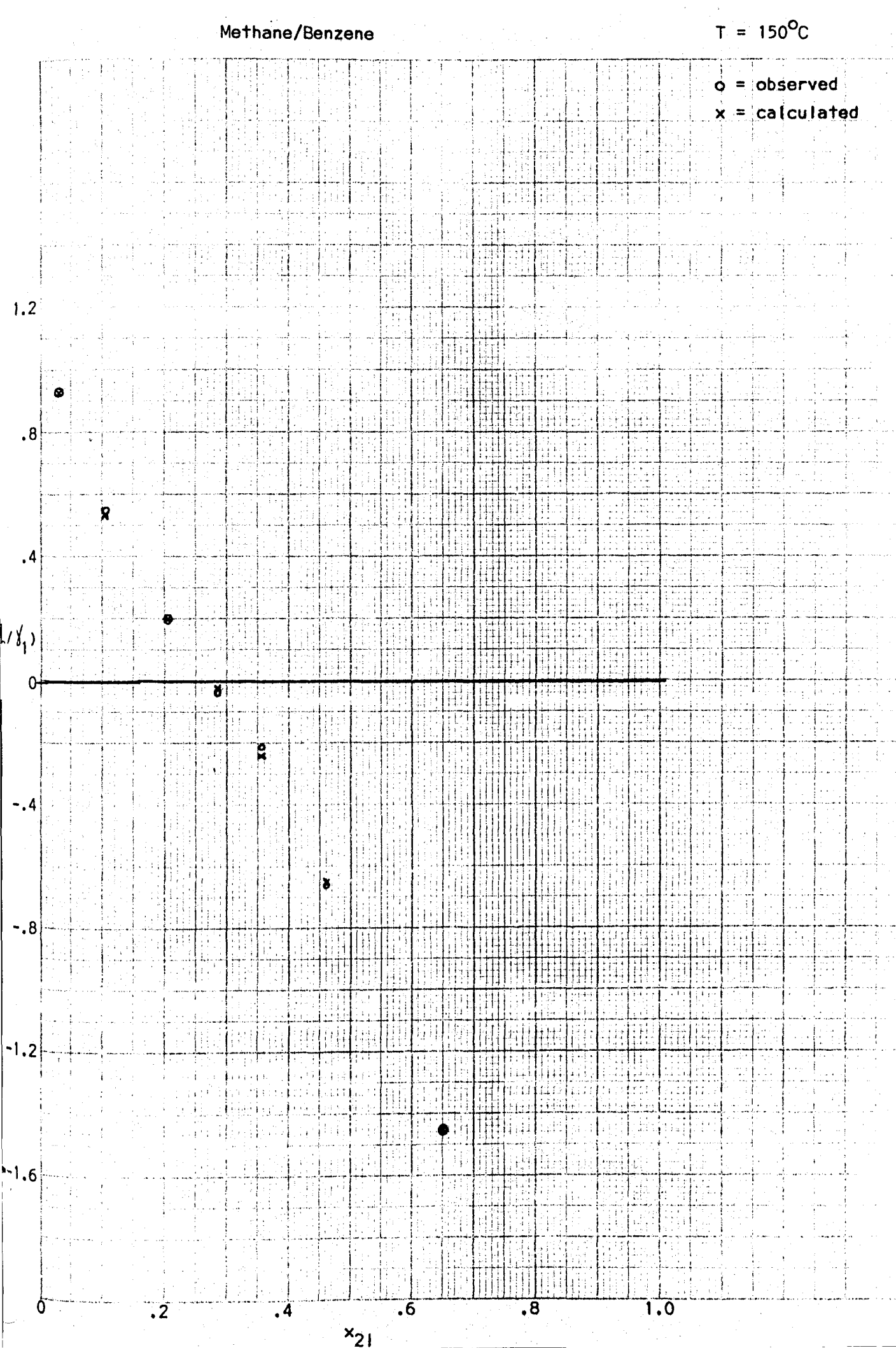
P_2 CALC.	DIF.
252.2295	58.7954
882.8033	92.6840
1723.5683	-97.7562
2396.1803	16.0300
2984.7158	213.8927
3867.5191	-156.4263

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.1542	0.0543	21.2463	0.9320	-0.0035
1	-8.1767	1.3140	-6.2229	0.5357	0.0092
2	27.2611	8.5327	3.1949	0.2050	-0.0020
3	-56.2158	19.9914	-2.8120	-0.0180	-0.0241
4	37.1651	15.1159	2.4587	-0.2377	0.0296
				-0.6464	-0.0100
				-1.4469	0.0008

Degrees of Freedom= 2
Integral at x=1: -0.4680
Error in Integral: 0.0136


Methane/Benzene
T = 150°C
o = observed
x = calculated
2000
1500
1000
500
0
.2
.4
.6
.8
1.0
x_{21}


Methane/Benzene
T = 150°C
o = observed
x = calculated
1.2
.8
.4
0
-.4
-.8
-1.2
-1.6
0
.2
.4
.6
.8
1.0
x_{21}

System: Propane/Benzene T= 38°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

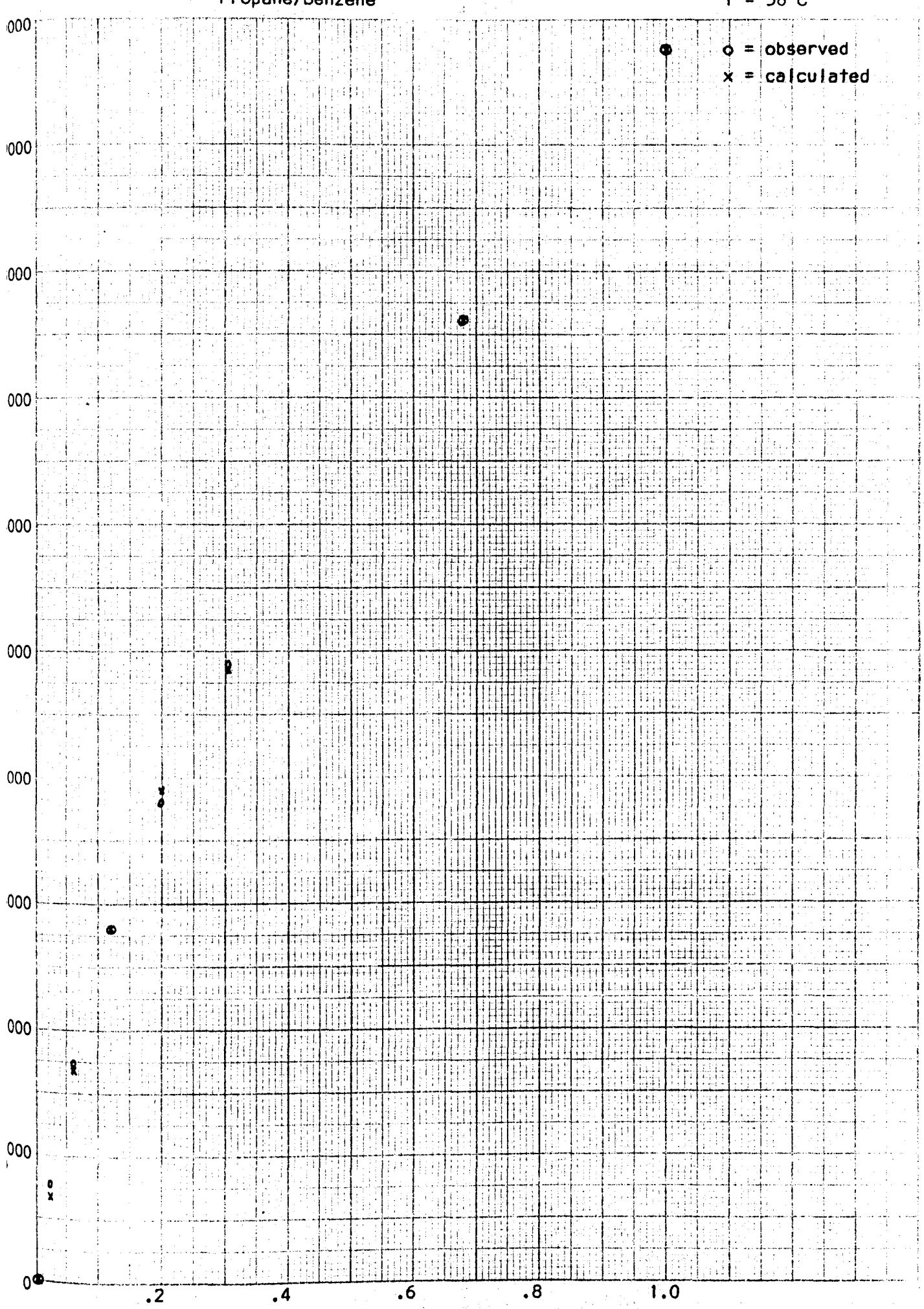
P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
167.20	0.0000	0.0000	0.0000	1.0000	1.0000	------
1064.00	0.0228	0.7378	785.0192	3.5283	1.7075	0.3152
2052.00	0.0624	0.8490	1742.1480	2.8610	1.9765	0.1606
3116.00	0.1194	0.9000	2804.4000	2.4069	2.1163	0.0559
4104.00	0.1980	0.9310	3820.8240	1.9775	2.1118	-0.0285
5168.00	0.3038	0.9505	4912.1840	1.6569	2.1976	-0.1226
7752.00	0.6801	0.9831	7620.9912	1.1483	2.4493	-0.3290
9758.40	1.0000	1.0000	9758.4000	1.0000	1.0000	------

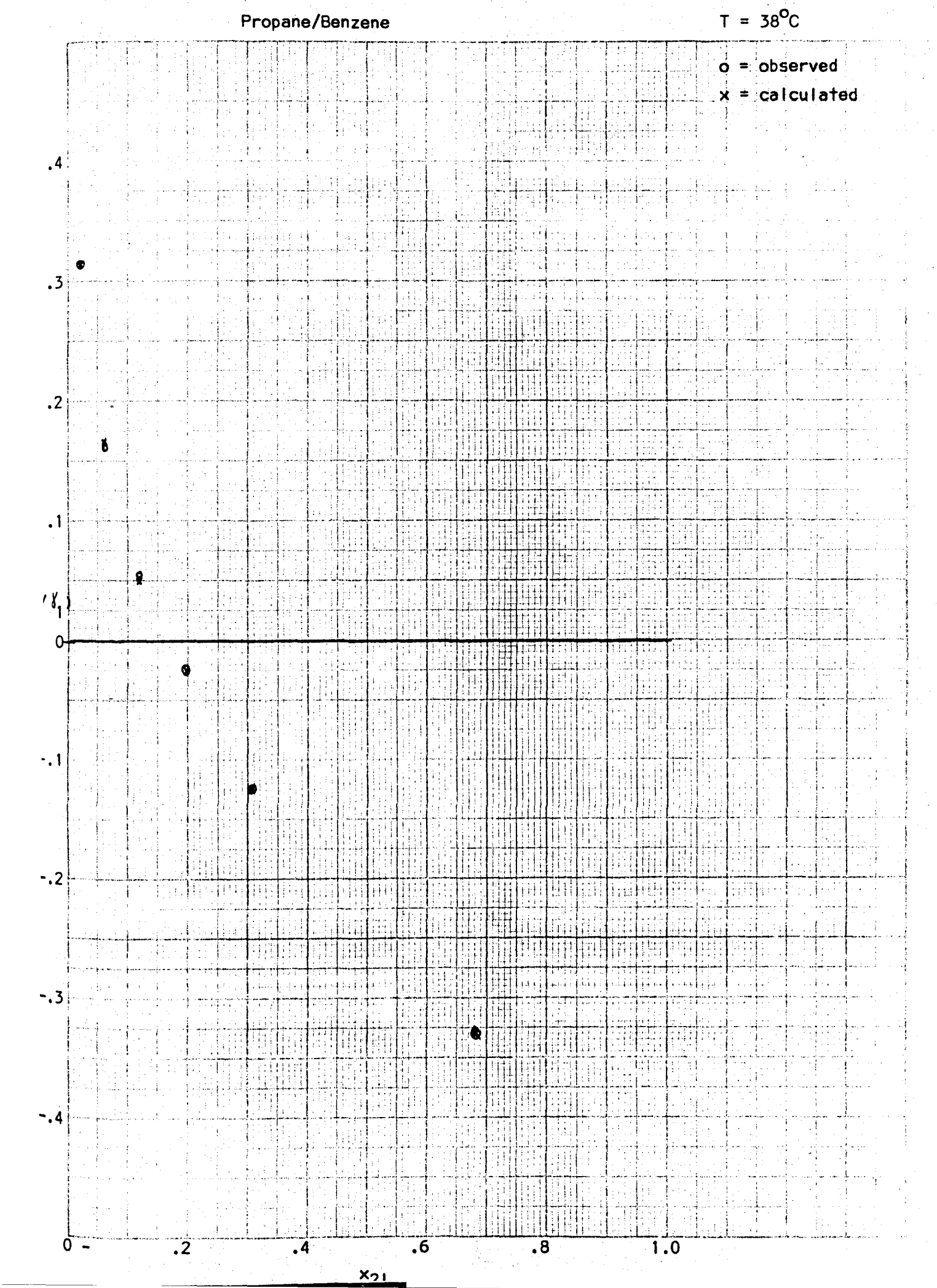
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	31512.5793	1115.8575	28.2407	0.0000	0.0000
2	-77518.4441	7616.8388	-10.1772	679.3693	105.6498
3	100558.2675	13983.6493	7.1911	1688.3003	53.8477
4	-44794.7372	7487.7398	-5.9824	2819.5381	-15.1381
				3912.1829	-91.3589
Degrees of Freedom: 4				4856.9852	55.1988
Confidence in First Term= 99.5%+				7625.9556	-4.9644
Confidence in Last Term= 99.5%+				9757.6655	0.7345

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.4509	0.0200	21.5458	------	------
1	-5.8178	0.6703	-8.6790	0.3129	0.0023
2	29.6939	5.9635	4.9793	0.1670	-0.0064
3	-71.4002	17.9609	-3.9753	0.0494	0.0065
4	55.7293	15.5865	3.5755	-0.0255	-0.0031
				-0.1232	0.0006
Degrees of Freedom: 1				-0.3290	0.0000
Integral at x=1: 0.7158				-------	------
Error in Integral: 0.0041					


Propane/Benzene
T = 38°C
o = observed
x = calculated
.2
.4
.6
.8
1.0


Propane/Benzene
T = 38°C
o = observed
x = calculated
.4
.3
.2
.1
0
-.1
-.2
-.3
-.4
γ_1
0
.2
.4
.6
.8
1.0
x_{21}

System: Propane/Benzene T= 71°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerma

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
577.60	0.0000	0.0000	0.0000	1.0000	1.0000	------
1064.00	0.0076	0.3046	324.0944	2.1482	1.2908	0.2212
2052.00	0.0277	0.6114	1254.5928	2.2816	1.4199	0.2060
3116.00	0.0495	0.7420	2312.0720	2.3529	1.4643	0.2060
4104.00	0.0772	0.7980	3274.9920	2.1370	1.5553	0.1380
5168.00	0.1083	0.8280	4279.1040	1.9904	1.7259	0.0619
7752.00	0.2107	0.8780	6806.2560	1.6273	2.0745	-0.1054
10336.00	0.3453	0.9172	9480.1792	1.3830	2.2631	-0.2139
12920.00	0.5146	0.9481	12249.4520	1.1991	2.3917	-0.2998
15504.00	0.7023	0.9727	15080.7408	1.0817	2.4615	-0.3571
18088.00	0.8801	0.9903	17912.5464	1.0253	2.5335	-0.3929
19851.20	1.0000	1.0000	19851.2000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	49741.0674	1033.1656	48.1443
2	-114152.0776	9333.6138	-12.2303
3	191580.3830	28057.6082	6.8281
4	-158888.2343	33726.9144	-4.7110
5	51583.1678	14022.2923	3.6787

Degrees of Freedom= 7
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

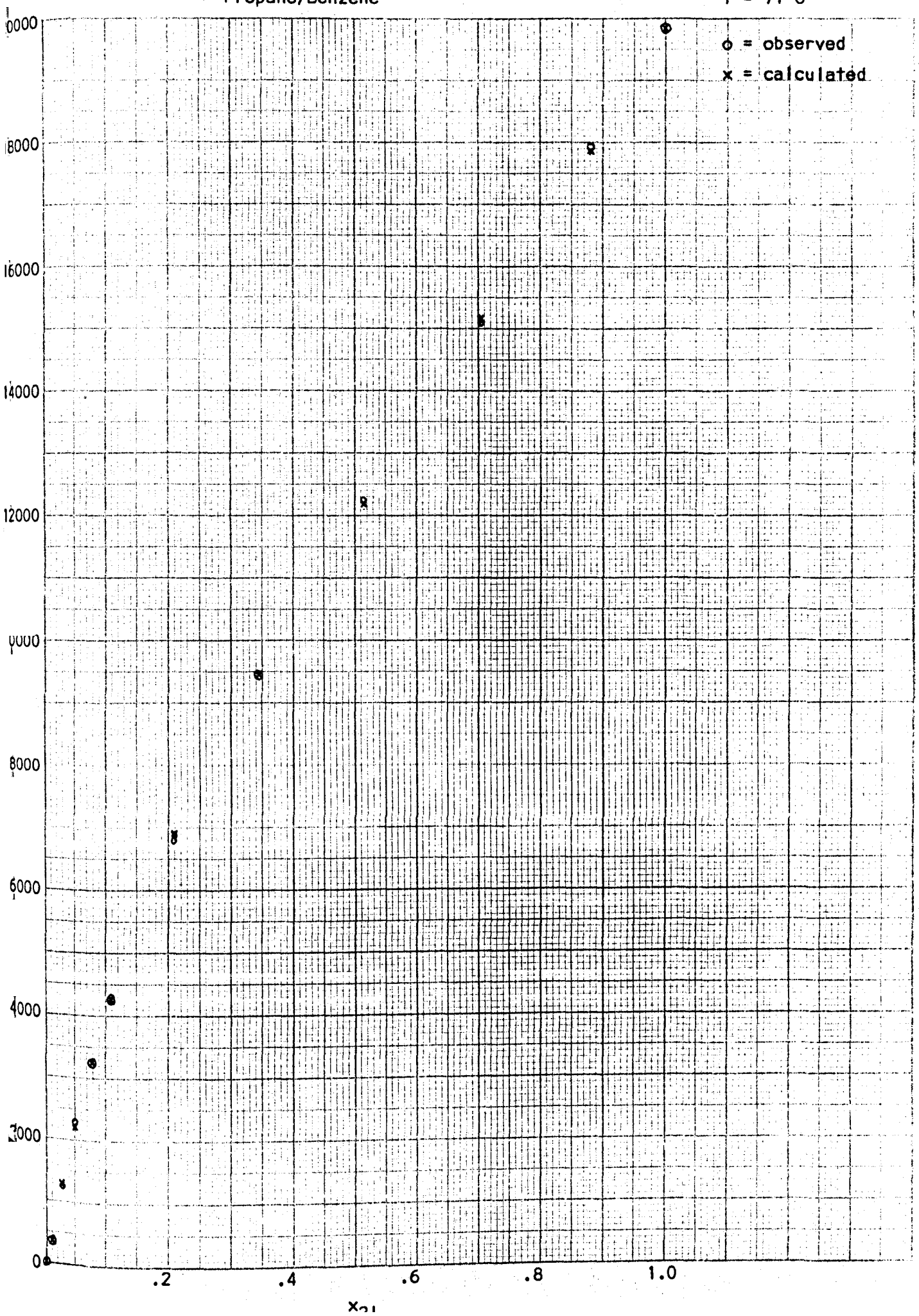
P_2 CALC.	DIF.
0.0000	0.0000
371.5223	-47.4279
1294.2190	-39.6262
2204.7794	107.2926
3242.3261	32.6659
4270.3440	8.7600
6913.0194	-106.7634
9446.9396	33.2396
12194.2620	55.1900
15152.4168	-71.6760
17868.5315	44.0149
19864.3062	-13.1062

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.2466	0.0171	14.4399
1	-1.6781	0.1263	-13.2833
2	1.1085	0.1473	7.5272

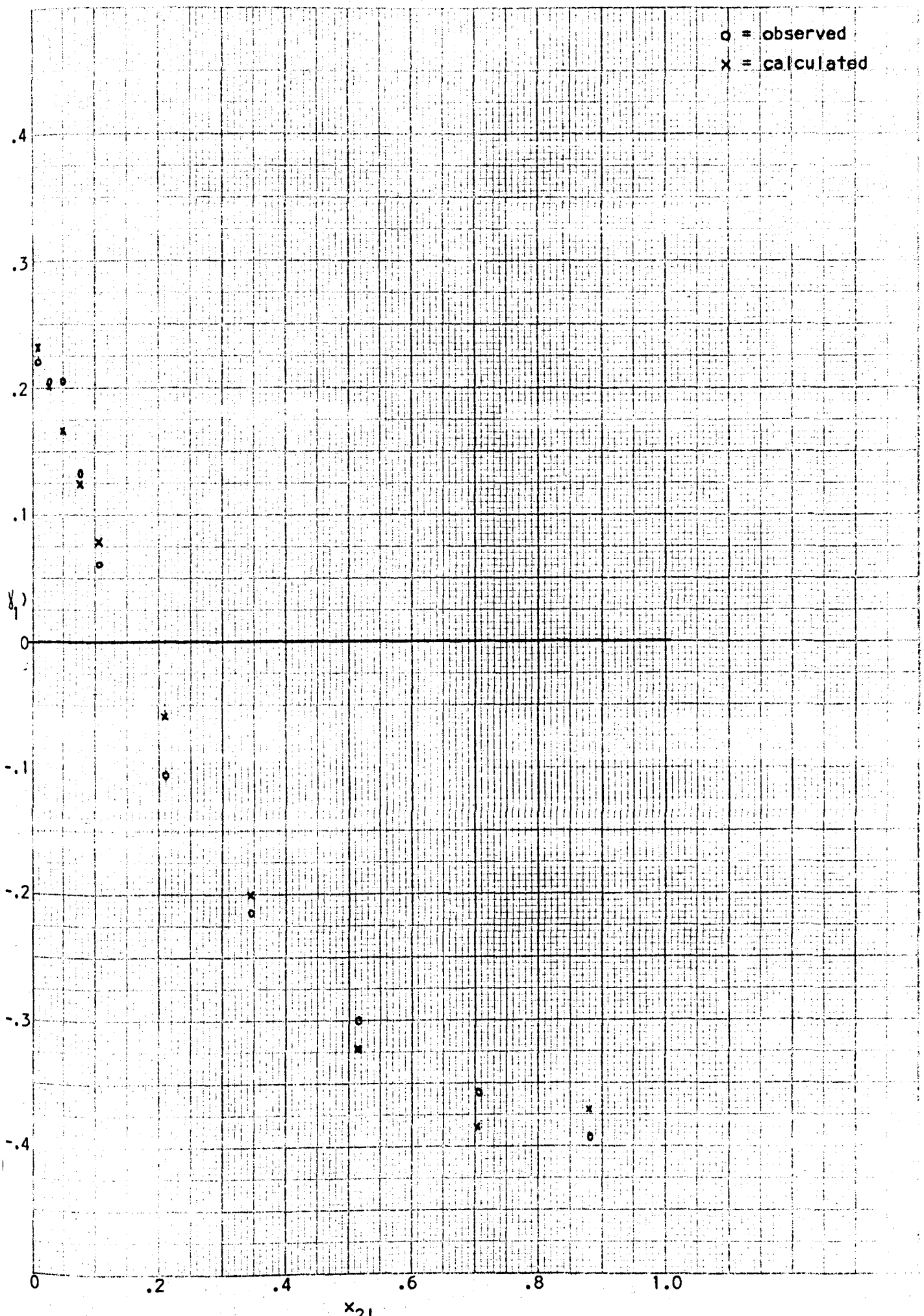
Degrees of Freedom= 7
Integral at x=1: -0.2230
Error in Integral: 0.0254

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
------	------
0.2339	-0.0127
0.2010	0.0050
0.1663	0.0397
0.1237	0.0143
0.0779	-0.0159
-0.0578	-0.0477
-0.2007	-0.0132
-0.3234	0.0236
-0.3852	0.0281
-0.3717	-0.0212
------	------


Propane/Benzene
T = 71°C
ϕ = observed
x = calculated
0000
8000
16000
14000
12000
9000
8000
6000
4000
3000
0
.2
.4
.6
.8
1.0
x_{21}

Propane/Benzene

T = 71°C



System: Propane/Benzene T= 104°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
1512.40	0.0000	0.0000	0.0000	1.0000	1.0000	------
2052.00	0.0074	0.1670	342.6840	1.3803	1.1386	0.0836
3116.00	0.0220	0.3596	1120.5136	1.5181	1.3491	0.0512
4104.00	0.0376	0.4772	1958.4288	1.5525	1.4741	0.0225
5168.00	0.0533	0.5573	2880.1264	1.6106	1.5979	0.0034
7752.00	0.1015	0.6792	5265.1584	1.5462	1.8301	-0.0732
10336.00	0.1572	0.7507	7759.2352	1.4712	2.0215	-0.1380
12920.00	0.2227	0.7997	10332.1240	1.3829	2.2013	-0.2019
15504.00	0.2945	0.8371	12978.3984	1.3135	2.3670	-0.2557
18088.00	0.3749	0.8642	15631.6496	1.2428	2.5982	-0.3202
20672.00	0.4640	0.8920	18439.4240	1.1845	2.7541	-0.3664
23256.00	0.5671	0.9144	21265.2864	1.1177	3.0406	-0.4346
25840.00	0.6675	0.9313	24064.7920	1.0746	3.5301	-0.5165
28424.00	0.7657	0.9467	26909.0008	1.0475	4.2754	-0.6107
31008.00	0.8797	0.9622	29835.9876	1.0109	6.4422	-0.8042
33044.80	0.9740	0.9740	32185.6352	0.9849	21.8492	-1.3458

PARTIAL PRESSURE CURVE FITTING:

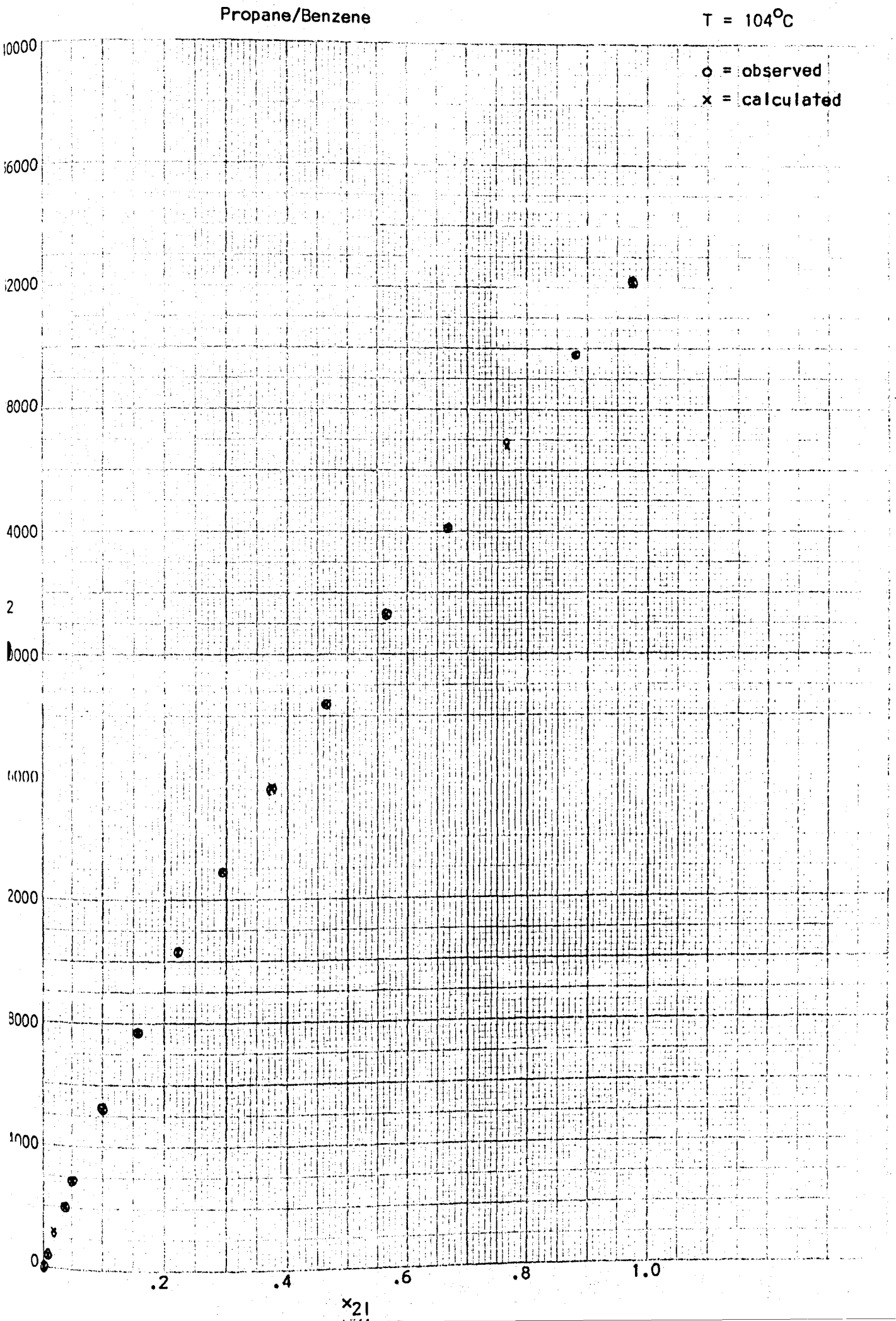
n	a_n	STD.ERROR	t
1	56932.5245	586.2945	97.1057
2	-57542.9131	3327.2036	-17.2947
3	51999.9512	5793.7751	8.9751
4	-18567.9469	3115.6936	-5.9595

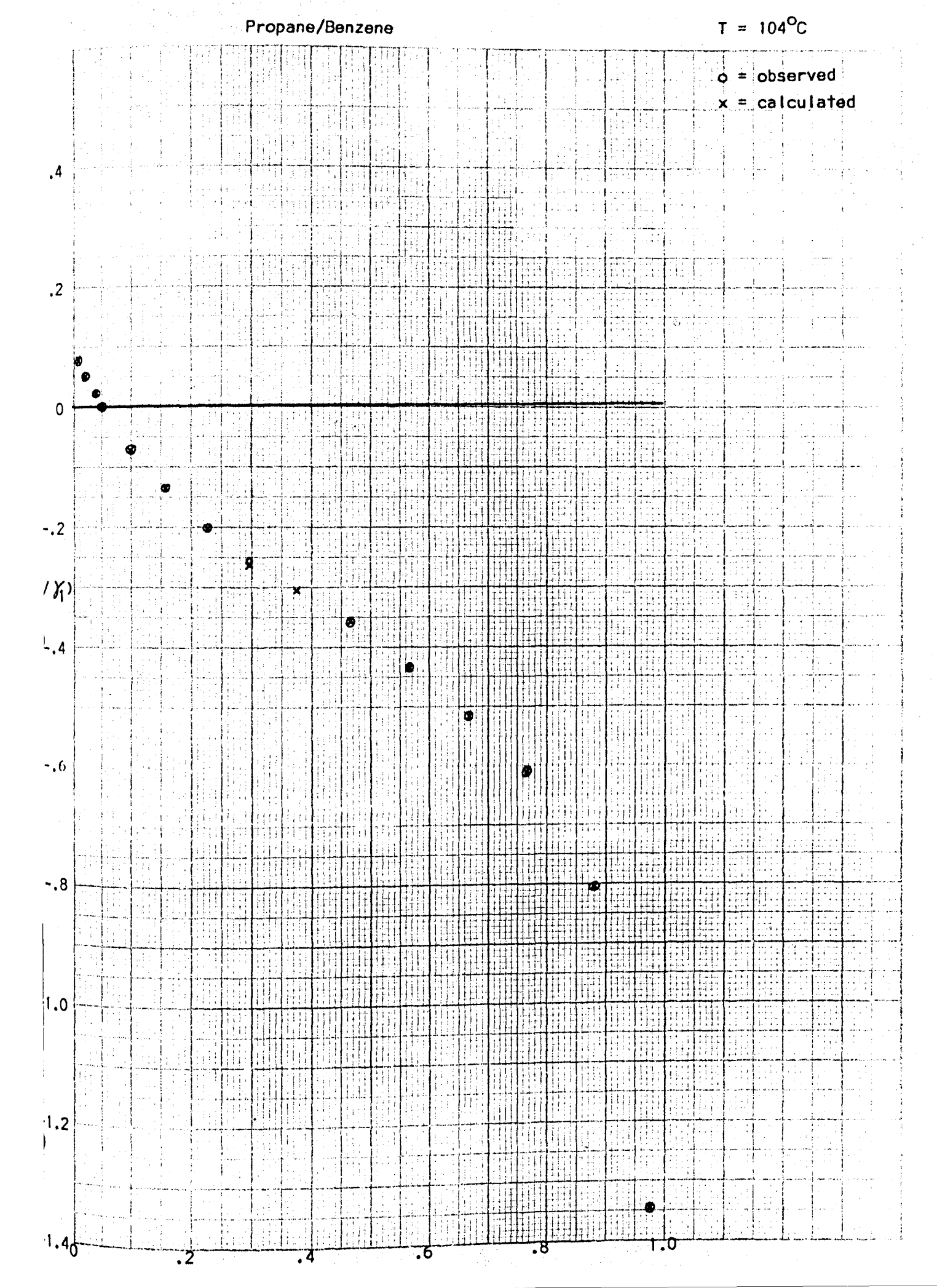
Degrees of Freedom= 12
Confidence In First Term= 99.5%+
Confidence In Last Term= 99.5%+

P_2 CALC.	DIF.
0.0000	0.0000
418.1706	-75.4866
1225.2141	-104.7005
2062.0381	-103.6093
2878.7544	1.3720
5238.2342	26.9242
7718.4669	40.7683
10353.6770	-21.5530
12964.4324	13.9660
15629.5413	2.1083
18361.9210	77.5030
21343.8363	-78.5499
24142.9827	-78.1907
26817.6072	91.3936
29833.0334	2.8642
32200.3001	-14.6649

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1008	0.0047	21.3293	------	------
1	-2.3936	0.2268	-10.5553	0.0837	-0.0001
2	10.9787	3.0312	3.6219	0.0529	-0.0017
3	-54.2158	17.2840	-3.1368	0.0238	-0.0013
4	169.0732	49.3001	3.4295	-0.0025	0.0060
5	-291.0441	73.8056	-3.9434	-0.0706	-0.0026
6	252.3689	55.3772	4.5573	-0.1358	-0.0021
7	-86.5130	16.4066	-5.2731	-0.2017	-0.0002
				-0.2616	0.0059
Degrees of Freedom= 7				-0.3151	-0.0051
Integral at x=1: -0.4455				-0.3669	0.0005
Error in Integral: 0.0028				-0.4352	0.0006
				-0.5173	0.0009
				-0.6094	-0.0013
				-0.8048	0.0006
				-1.3457	-0.0001


Propane/Benzene
T = 104°C
o = observed
x = calculated
10000
6000
2000
8000
4000
2
3000
6000
2000
3000
1000
0
.2
.4
.6
.8
1.0
x21


Propane/Benzene
T = 104°C
o = observed
x = calculated
.4
.2
0
-.2
-.4
-.6
-.8
1.0
1.2
1.4
0
.2
.4
.6
.8
1.0

System: Propane/Benzene T= 138°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
3344.00	0.0000	0.0000	010000	1.0000	1.0000	------
4104.00	0.0081	0.1108	454.7232	1.3463	1.1002	0.0876
5168.00	0.0190	0.2206	1140.0608	1.4389	1.2279	0.0689
7752.00	0.0479	0.3992	3094.5984	1.5493	1.4628	0.0249
10336.00	0.0792	0.5077	5247.5872	1.5889	1.6525	-0.0170
12920.00	0.1133	0.5819	7518.1480	1.5913	1.8218	-0.0587
15504.00	0.1503	0.6352	9848.1408	1.5713	1.9905	-0.1027
18088.00	0.1906	0.6750	12209.4000	1.5362	2.1719	-0.1504
20672.00	0.2340	0.7047	14567.5584	1.4929	2.3831	-0.2031
23256.00	0.2768	0.7255	16872.2280	1.4617	2.6397	-0.2566
25840.00	0.3292	0.7474	19312.8160	1.4069	2.9098	-0.3156
28424.00	0.3913	0.7645	21730.1480	1.3304	3.2907	-0.3932
31008.00	0.4574	0.7814	24229.6512	1.2703	3.7358	-0.4684
33668.00	0.5261	0.7991	26904.0988	1.2263	4.2682	-0.5415
36176.00	0.6113	0.8052	29128.9152	1.1427	5.4216	-0.6761
38760.00	0.7104	0.8084	31333.5840	1.0577	7.6666	-0.8602
39770.80	0.7980	0.7980	31737.0984	0.9537	11.8932	-1.0957

PARTIAL PRESSURE CURVE FITTING:

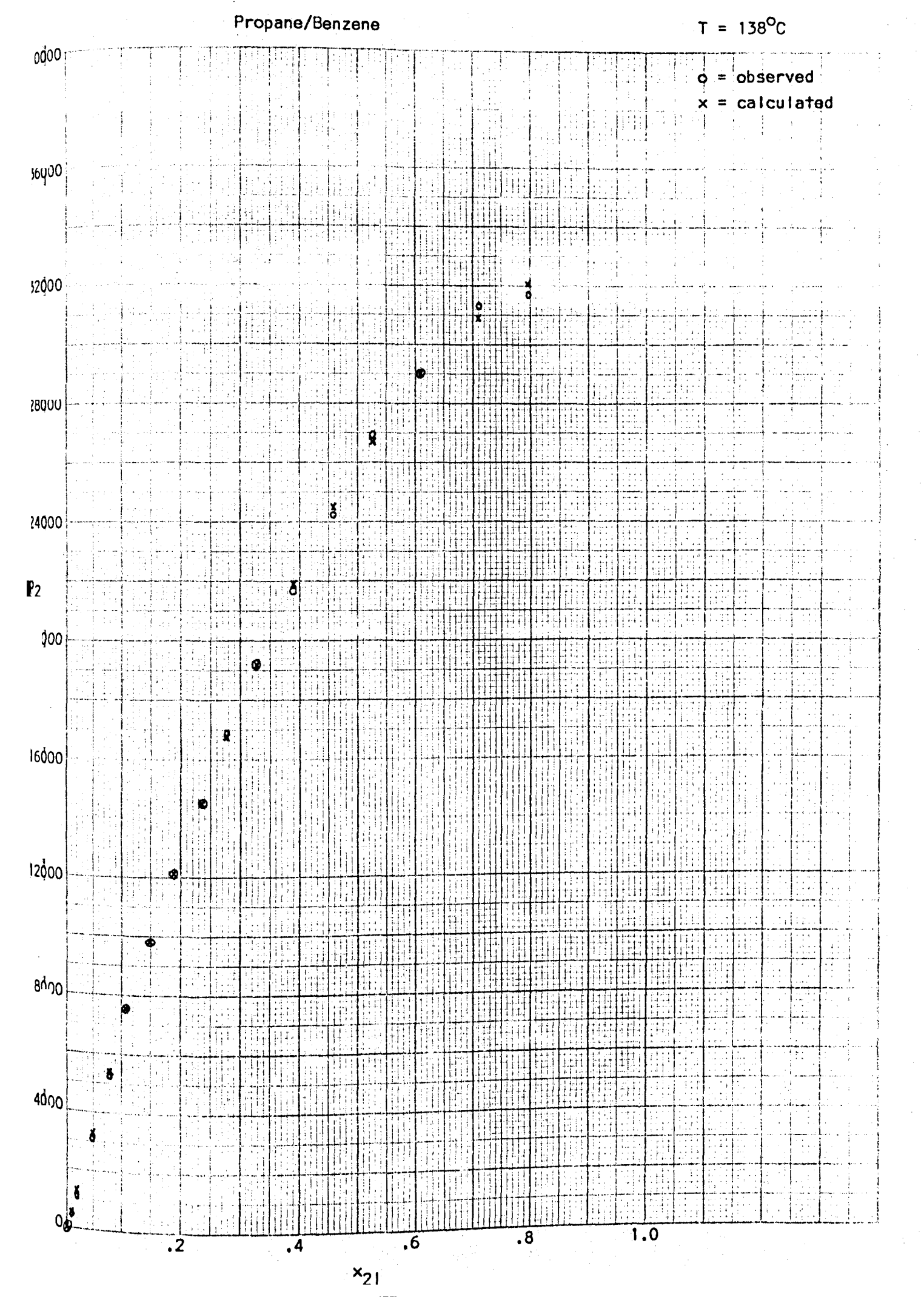
n	a_n	STD.ERROR	t
1	71314.9952	411.4236	173.3372
2	-39012.6130	658.4156	-59.2523

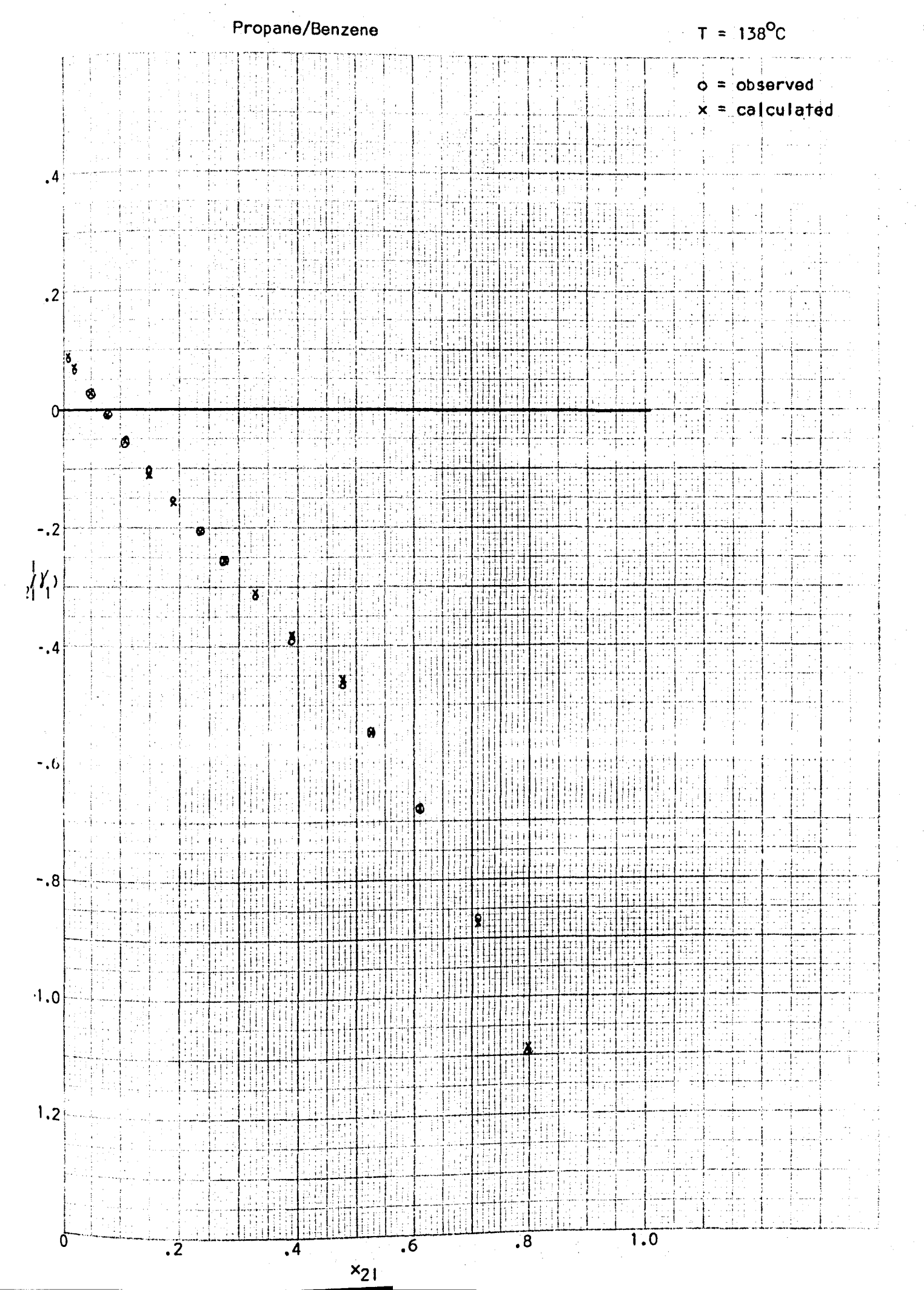
Degrees of Freedom= 15
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

P_2 CALC.	DIF.
- 0.0000	0.0000
575.0918	-120.3686
1340.9014	-200.8406
3326.4773	-231.8789
5403.4355	-155.8483
7579.1883	-61.0403
9837.3453	10.7955
12175.3738	34.0262
14551.5342	16.0242
16750.9129	121.3151
19248.9966	63.8194
21948.4217	-218.2737
24457.4644	-227.8132
26720.8608	183.2380
29016.3234	112.5918
30973.7490	359.8350
32065.9782	-328.8798

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1036	0.0056	18.4772	------	------
1	-1.6686	0.0714	-23.3548	0.0902	-0.0026
2	1.9610	0.2243	8.7439	0.0726	-0.0037
3	-2.1781	0.1894	-11.5021	0.0279	-0.0030
				-0.0173	0.0003
Degrees of Freedom= 12				-0.0635	0.0047
Integral at x=1: -0.6216				-0.1103	0.0076
Error in Integral: 0.0072				-0.1583	0.0079
				-0.2074	0.0043
				-0.2542	-0.0024
				-0.3109	-0.0047
				-0.3800	-0.0132
				-0.4578	-0.0106
				-0.5486	0.0071
				-0.6812	0.0051
				-0.8730	0.0128
				-1.0860	-0.0097


Propane/Benzene
T = 138°C
o = observed
x = calculated
P2
x21
.2
.4
.6
.8
1.0


Propane/Benzene
T = 138°C
o = observed
x = calculated
.4
.2
0
-.2
-.4
-.6
-.8
1.0
1.2
ln(γ1)
0
.2
.4
.6
.8
1.0
x21

System: Propane/Benzene T= 171°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
6513.20	0.0000	0.0000	0.0000	1.0000	1.0000	------
7752.00	0.0103	0.1923	1490.7096	3.0027	0.9713	0.4901
10336.00	0.0323	0.2332	2410.3552	1.5482	1.2575	0.0903
12920.00	0.0552	0.3304	4268.7680	1.6044	1.4059	0.0574
15504.00	0.0793	0.4030	6248.1120	1.6347	1.5435	0.0249
18088.00	0.1048	0.4588	8298.7744	1.6429	1.6789	-0.0094
20672.00	0.1312	0.5022	10381.4784	1.6416	1.8185	-0.0444
23256.00	0.1600	0.5362	12469.8672	1.6169	1.9715	-0.0861
25840.00	0.1905	0.5650	14599.6000	1.5900	2.1319	-0.1273
28424.00	0.2234	0.5848	16622.3552	1.5437	2.3332	-0.1794
31008.00	0.2276	0.6042	18735.0336	1.7078	2.4396	-0.1548
33592.00	0.2917	0.6185	20776.6520	1.4777	2.7779	-0.2741
36176.00	0.3358	0.6266	22667.8816	1.4005	3.1225	-0.3482
38760.00	0.3794	0.6278	24333.5280	1.3306	3.5691	-0.4284
41344.00	0.4290	0.6227	25744.9088	1.2451	4.1944	-0.5274
43928.00	0.4968	0.5773	25359.6344	1.0590	5.6655	-0.7282
44422.00	0.5490	0.5490	24387.6780	0.9216	6.8203	-0.8691

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	90916.6476	2414.1482	37.6599
2	-70157.8372	7186.7888	-9.7621

Degrees of Freedom= 13
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

P_2 CALC.	DIF.
0.0000	0.0000
928.9984	561.7112
2863.4127	-453.0575
4804.8252	-536.0572
6768.5033	-520.3913
8757.5183	-458.7439
10720.6064	-339.1280
12750.6230	-280.7558
14773.5759	-173.9759
16809.3726	-187,0174
17058.3295	1676.7041
20550.7336	225.9184
22618.6965	49.1841
24394.9511	-61.4231
26091.3233	-346.4145
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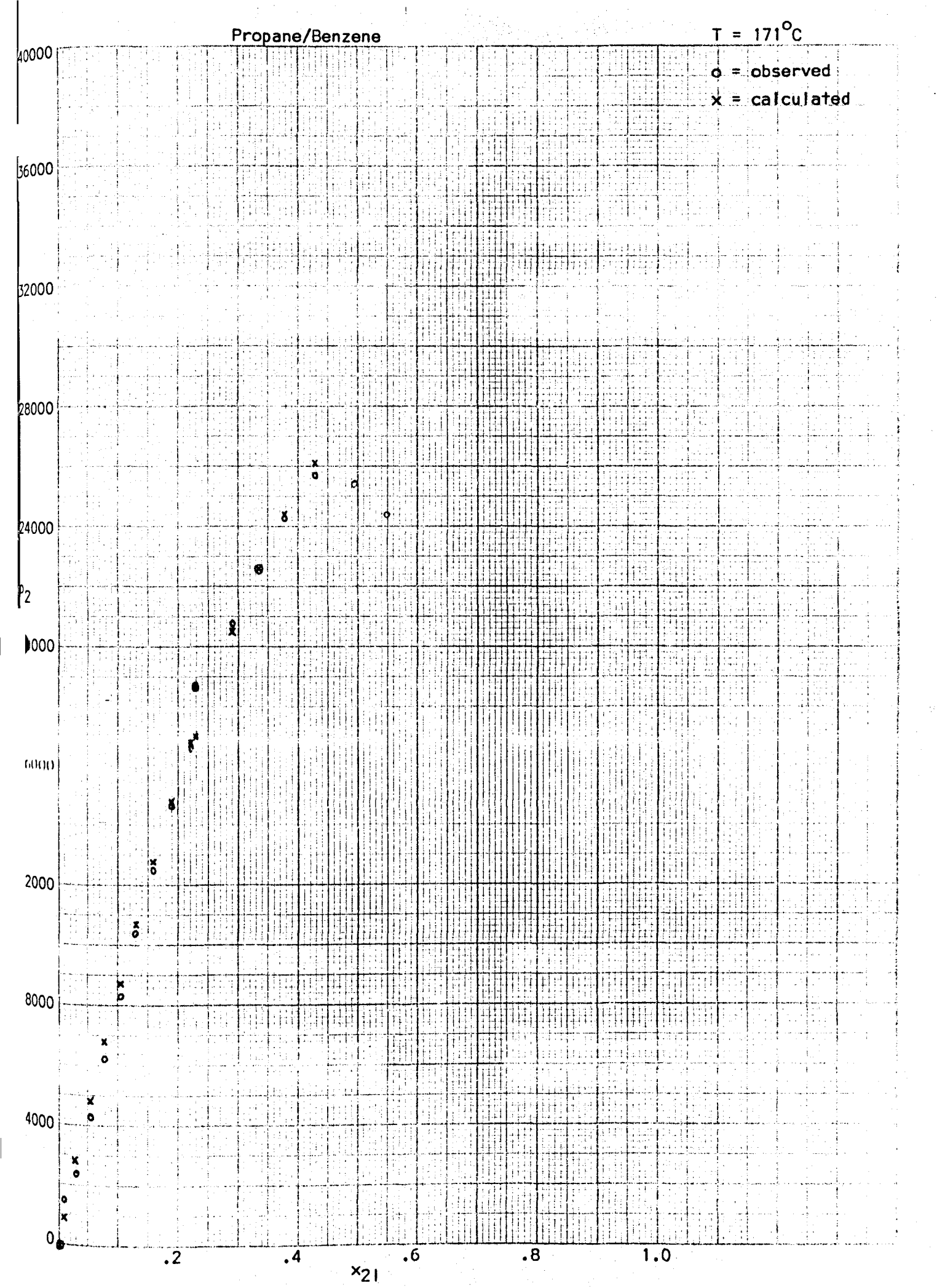
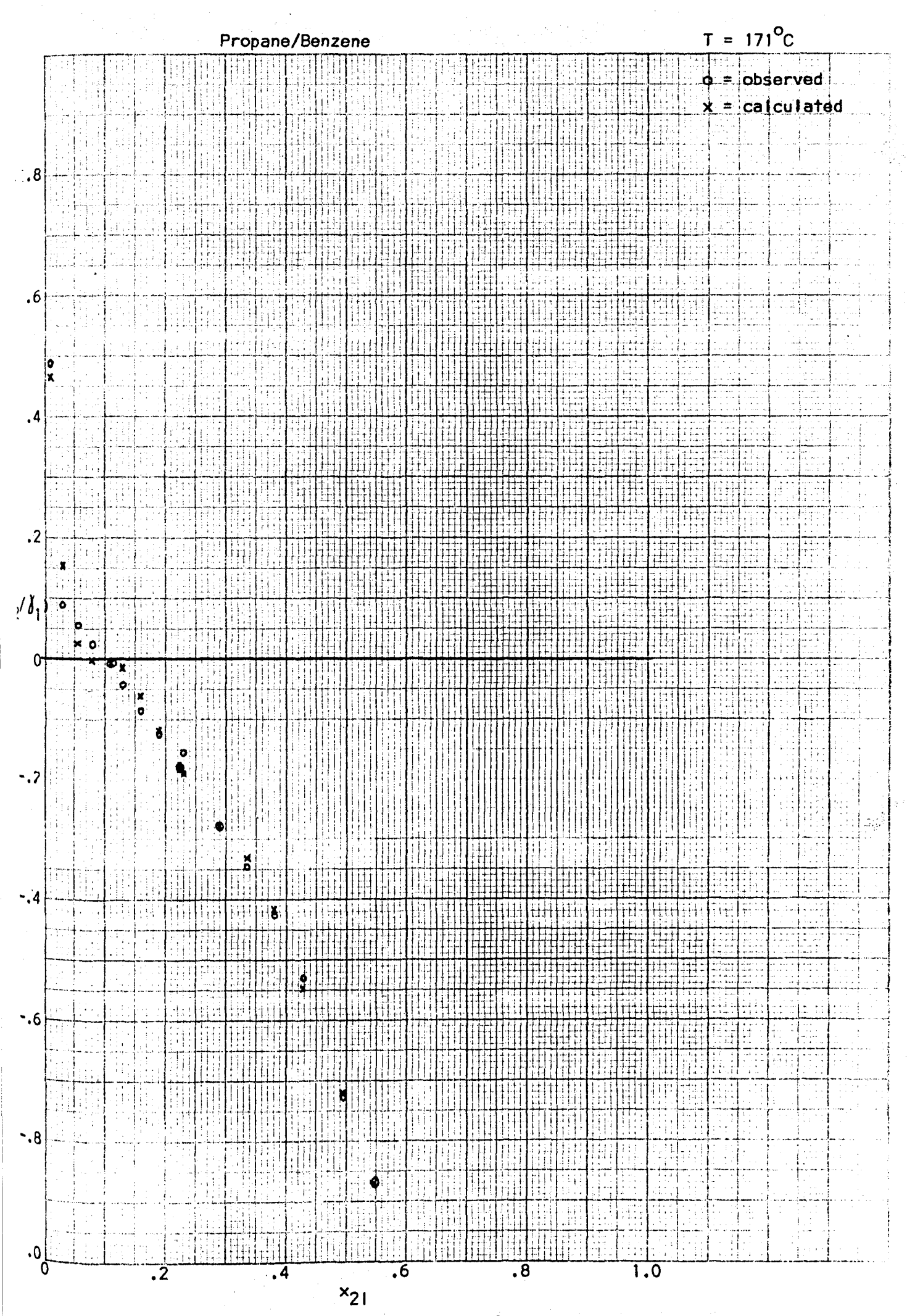
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.7168	0.0644	11.1359	------	------
1	-28.4878	4.4988	-6.3323	0.4665	0.0236
2	439.7926	96.9776	4.5350	0.1551	-0.0647
3	-3402.4611	923.4956	-3.6843	0.0274	0.0300
4	14073.0020	4494.8482	3.1309	-0.0080	0.0329
5	-31891.9373	11641.2808	-2.7396	-0.0134	0.0040
6	37276.3111	15241.6006	2.4457	-0.0261	-0.0183
7	-17564.3615	7922.2540	-2.2171	-0.0620	-0.0241
				-0.1178	-0.0095
Degrees of Freedom= 8				-0.1810	0.0016
Integral at x=1: -88.6252				-0.1884	0.0336
Error in Integral: 0.0248				-0.2781	0.0040
				-0.3335	-0.0146
				-0.4158	-0.0126
				-0.5485	0.0211
				-0.7196	-0.0086
				-0.8709	0.0018


Propane/Benzene
T = 171°C
o = observed
x = calculated
40000
36000
32000
28000
24000
P2
8000
2000
8000
4000
0
.2
.4
.6
.8
1.0
x21


Propane/Benzene
T = 171°C
o = observed
x = calculated
.8
.6
.4
.2
0
-.2
-.4
-.6
-.8
-1.0
0
.2
.4
.6
.8
1.0
x_{21}

System: Propane/Benzene T= 204°C.

Reference: Physico-Chemical Constants of Binary Systems, Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
11483.60	0.0000	0.0000	0.0000	1.0000	1.0000	------
12920.00	0.0097	0.0571	737.7320	1.5521	1.0712	0.1610
15504.00	0.0283	0.1456	2257.3824	1.6279	1.1871	0.1371
18088.00	0.0450	0.2059	3724.3192	1.6890	1.3097	0.1104
20672.00	0.0691	0.2588	5349.9136	1.5801	1.4333	0.0423
23256.00	0.0866	0.3062	7120.9872	1.6781	1.5383	0.0378
25840.00	0.1053	0.3384	8744.2560	1.6947	1.6639	0.0080
28424.00	0.1265	0.3685	10474.2440	1.6898	1.7894	-0.0249
31008.00	0.1500	0.3944	12229.5552	1.6639	1.9238	-0.0630
33592.00	0.1754	0.4184	14054.8928	1.6353	2.0632	-0.1009
36176.00	0.2027	0.4366	15794.4416	1.5902	2.2261	-0.1461
38760.00	0.2308	0.4461	17290.8360	1.5289	2.4305	-0.2013
41344.00	0.2597	0.4419	18269.9136	1.4357	2.7142	-0.2765
43928.00	0.3038	0.4132	18151.0496	1.2193	3.2242	-0.4222
44840.00	0.3490	0.3490	15649.1600	0.9151	3.9047	-0.6300

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	90831.7636	2252.1455	40.3312
2	-71650.7300	10898.3329	-6.5745

Degrees of Freedom= 11
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

P_2 CALC.	DIF.
0.0000	0.0000
874.3265	-136.5945
2513.1546	-255.7722
3942.3366	-218.0174
5934.3562	-584.4426
7328.6818	-207.6946
8770.1150	-25.8590
10343.6452	130.5988
12012.6231	216.9321
13727.5452	327.3476
15467.6642	326.7774
17147.2341	143.6019
18756.5907	-486.6771
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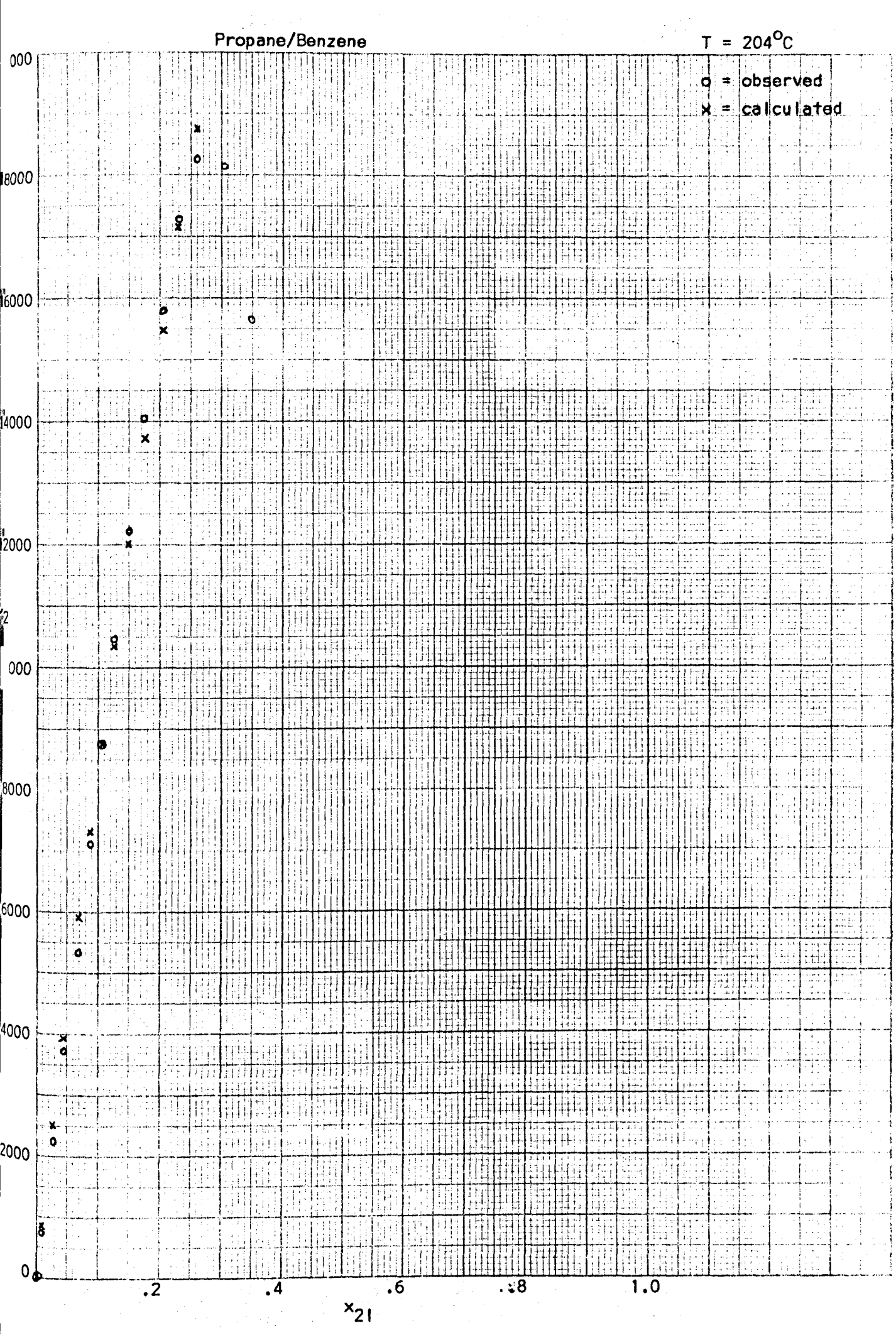
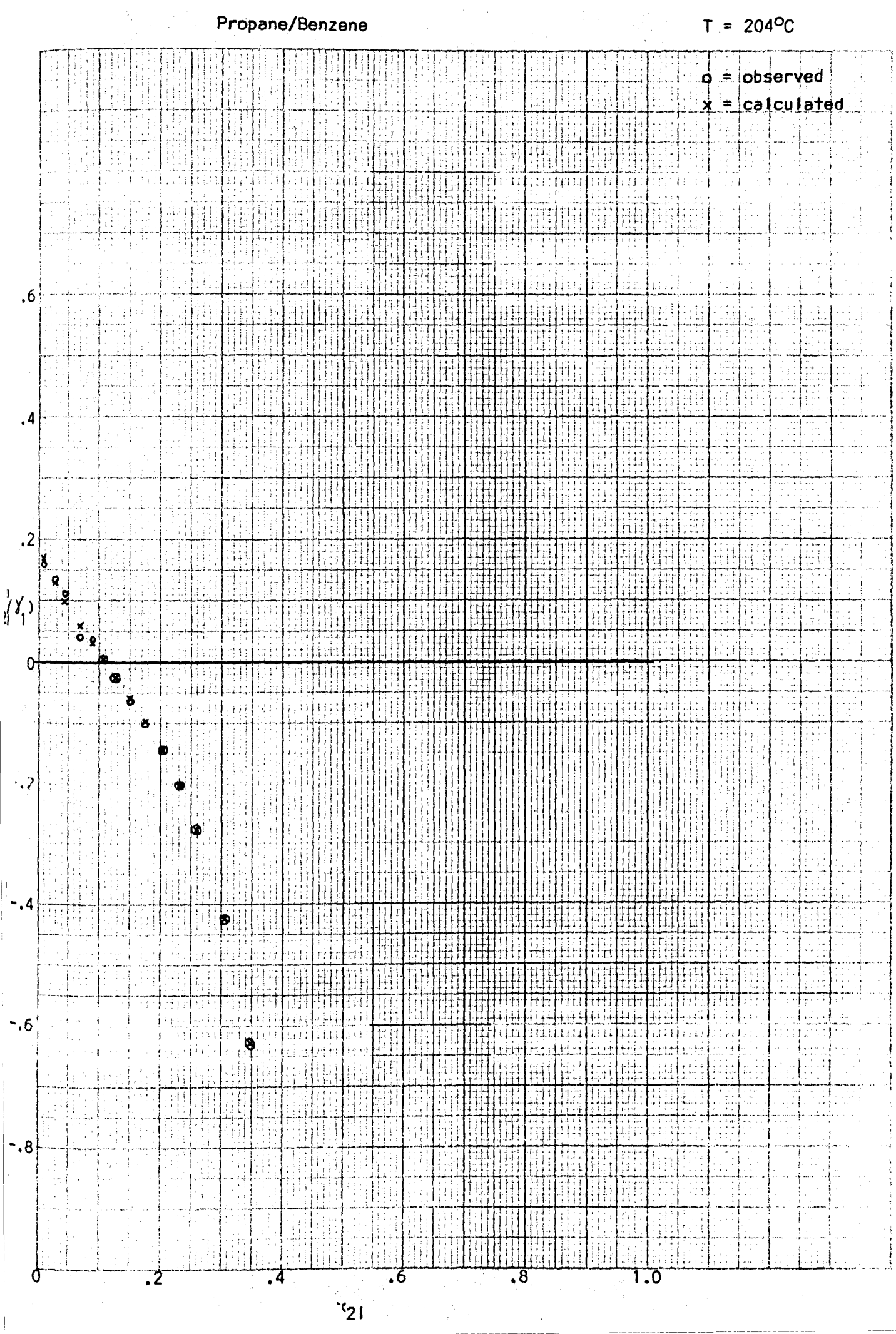
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1924	0.0075	25.7617	------	------
1	-2.4258	0.1893	-12.8165	0.1696	-0.0086
2	8.6452	1.2622	6.8495	0.1301	0.0070
3	-24.1609	2.3435	-10.3095	0.0985	0.0119
				0.0581	-0.0157
				0.0314	0.0063
				0.0046	0.0034
				-0.0251	0.0002
				-0.0585	-0.0045
				-0.0975	-0.0034
				-0.1453	-0.0007
				-0.2040	0.0027
				-0.2777	0.0012
				-0.4241	0.0019
				-0.6283	-0.0017

Degrees of Freedom= 10
Integral at x=1: -4.1790
Error in Integral: 0.0066


Propane/Benzene
T = 204°C
o = observed
x = calculated
000
8000
6000
4000
2000
0
.2
.4
.6
.8
1.0
x_{21}


Propane/Benzene
T = 204°C
o = observed
x = calculated
.6
.4
.2
0
-.2
-.4
-.6
-.8
0
.2
.4
.6
.8
1.0
γ_{21}

System: Heptane/Benzene T= 60°C.

Reference: Brown,Ewald(1951):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
216.43	0.9821	0.9578	207.3010	1.0027	1.3024	-0.1135
224.86	0.9546	0.9000	202.3830	1.0072	1.2625	-0.0981
239.66	0.9073	0.8070	193.4008	1.0127	1.2731	-0.0994
266.92	0.8121	0.6584	175.7268	1.0280	1.2386	-0.0819
294.35	0.7066	0.5283	155.5080	1.0454	1.2080	-0.0627
315.58	0.6129	0.4375	138.0536	1.0701	1.1704	-0.0389
335.65	0.5122	0.3543	118.9309	1.1030	1.1341	-0.0121
350.83	0.4216	0.2922	102.5055	1.1551	1.0957	0.0229
351.01	0.4198	0.2909	102.0913	1.1552	1.0951	0.0232
365.93	0.3164	0.2239	81.9390	1.2304	1.0603	0.0646
378.15	0.2088	0.1572	59.4263	1.3519	1.0282	0.1189
387.64	0.1042	0.0865	33.5154	1.5274	1.0010	0.1800
390.29	0.0575	0.0505	19.7214	1.6302	1.0035	0.2107
391.51	0.0210	0.0198	7.7480	1.7527	1.0005	0.2435

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	371.1529	2.6620	139.4263
2	-556.1616	22.1690	-25.0873
3	802.7162	64.5945	12.4270
4	-552.5984	77.1961	-7.1584
5	145.5617	32.3077	4.5055

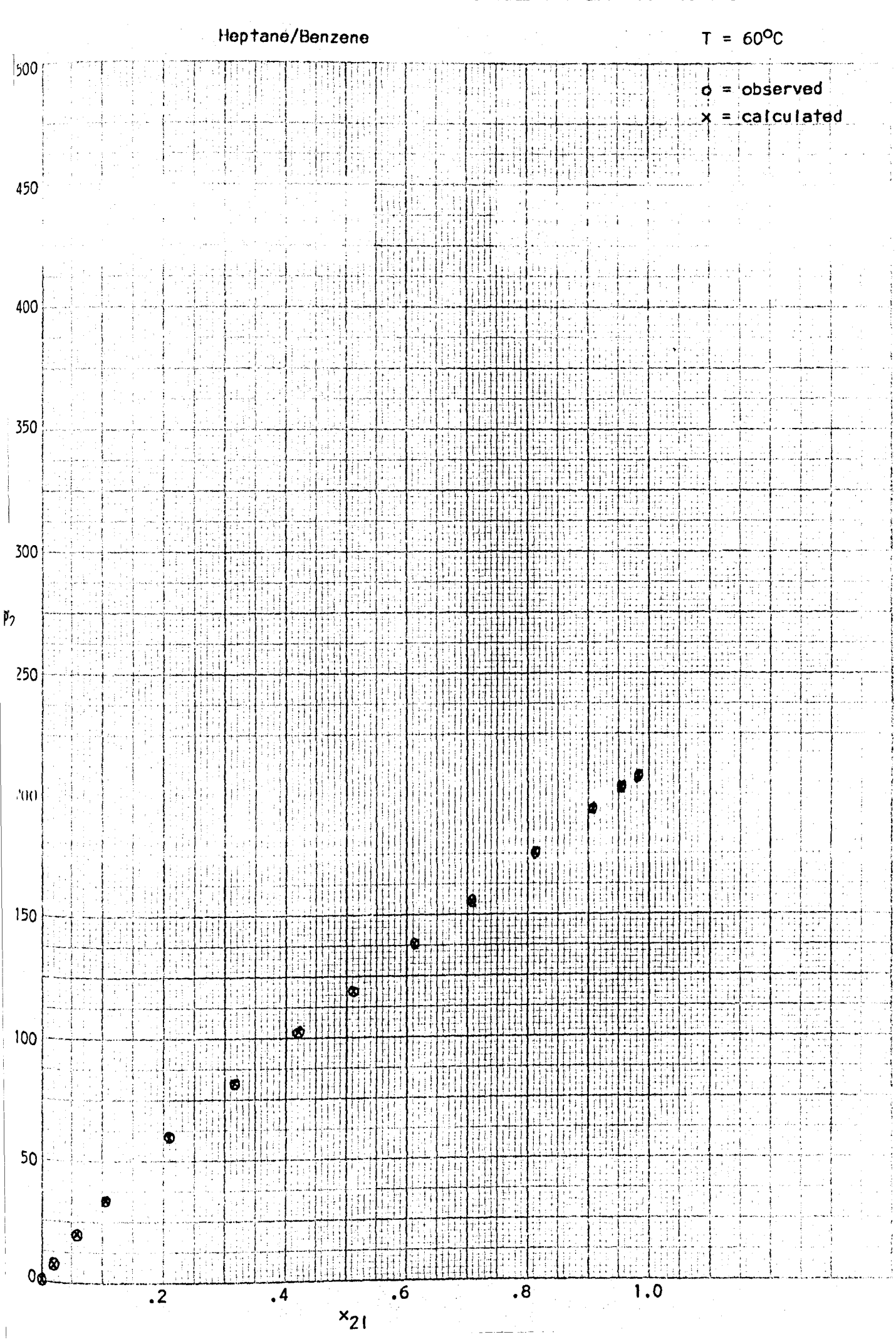
Degrees of Freedom= 10
Confidonce in First Term= 99.5%+
Confidonce in Last Term= 99.5%+

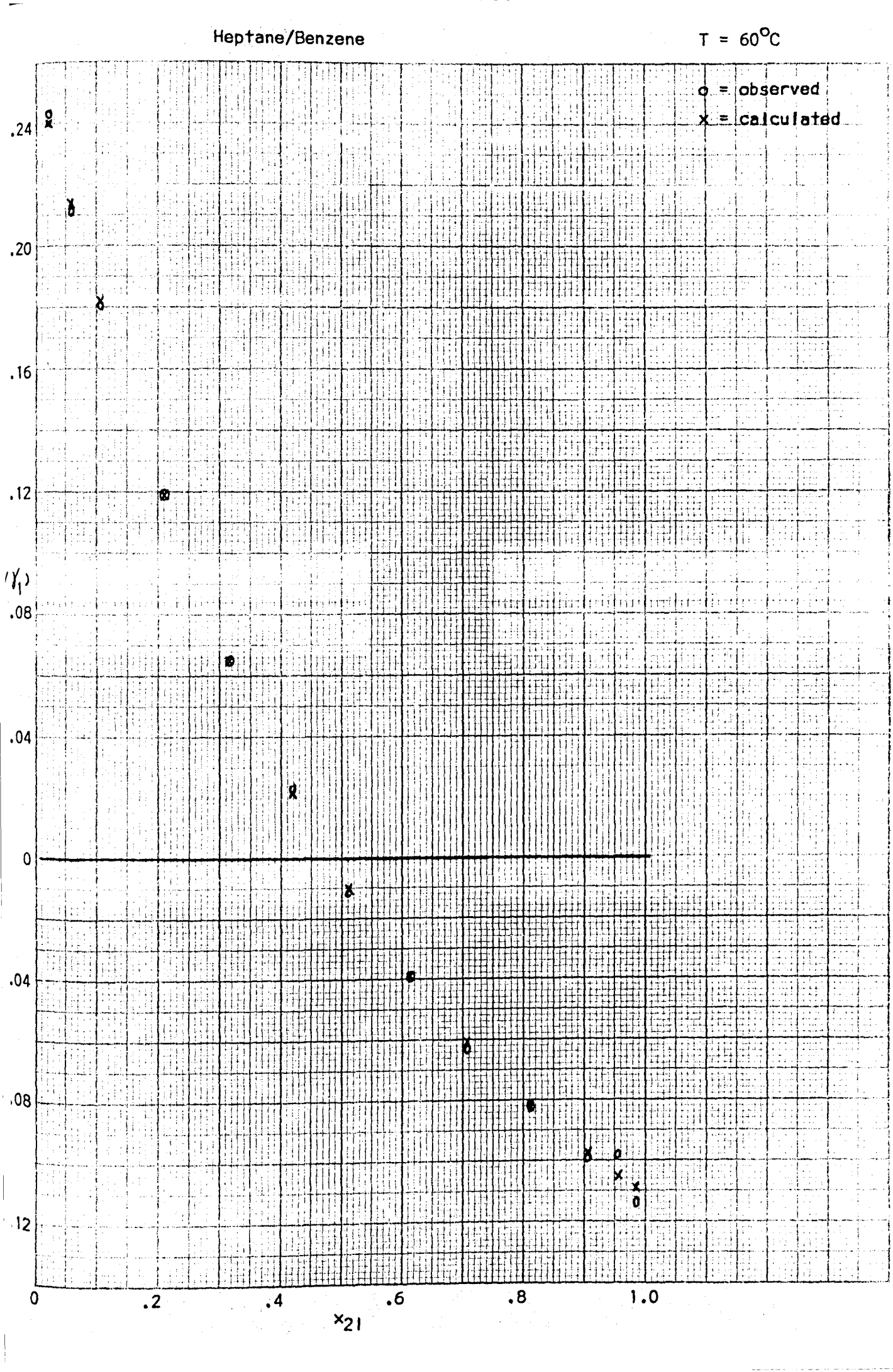
P_2 CALC.	DIF.
207.3693	-0.0683
202.2718	0.1112
193.4753	-0.0744
175.6039	0.1229
155.6610	-0.1530
137.9743	0.0794
119.1684	-0.2375
102.2488	0.2567
101.9242	0.1670
82.0973	-0.1582
59.5687	-0.1424
33.4915	0.0239
19.6397	0.0817
7.5563	0.1917

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.2562	0.0028	91.7796	-0.1090	-0.0046
1	-0.7744	0.0279	-27.7658	-0.1049	0.0068
2	0.5911	0.0684	8.6377	-0.0976	-0.0018
3	-0.1845	0.0452	-4.0837	-0.0817	0.0007
				-0.0609	-0.0018
				-0.0388	0.0000
				-0.0102	-0.0019
				0.0210	0.0020
				0.0216	0.0016
				0.0645	0.0001
				0.1186	0.0003
				0.1817	-0.0017
				0.2136	-0.0029
				0.2402	0.0033

Degrees of Freedom= 10
Integral at x=1: 0.0199
Error in Integral: 0.0028


Heptane/Benzene
T = 60°C
o = observed
x = calculated
500
450
400
350
300
250
200
150
100
50
0
p_2
.2
.4
.6
.8
1.0
x_{21}


Heptane/Benzene
T = 60°C
o = observed
x = calculated
.24
.20
.16
.12
(γ1)
.08
.04
0
.04
.08
.12
0
.2
.4
.6
.8
1.0
x21

System: Heptane/Benzene T= 80°C.

Reference: Brown,Ewald(1951):Physico-Chemical Constants of Binary Systems

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
440.14	0.9789	0.9571	421.2668	1.0055	1.1768	-0.0683
452.34	0.9556	0.9136	413.2533	1.0104	1.1606	-0.0602
453.06	0.9542	0.9099	412.2484	1.0094	1.1740	-0.0656
478.77	0.9071	0.8277	396.2731	1.0207	1.1704	-0.0594
527.72	0.8105	0.6776	357.5725	1.0307	1.1832	-0.0599
572.65	0.7117	0.5601	320.7184	1.0530	1.1511	-0.0387
614.60	0.6091	0.4554	279.8950	1.0736	1.1281	-0.0215
651.90	0.5048	0.3685	240.1991	1.1116	1.0955	0.0064
678.53	0.4181	0.3070	208.2884	1.1640	1.0647	0.0387
688.11	0.3842	0.2803	192.8772	1.1731	1.0595	0.0442
706.53	0.3152	0.2334	164.9041	1.2223	1.0421	0.0693
730.14	0.2079	0.1639	119.6407	1.3448	1.0154	0.1220
746.04	0.1168	0.0962	71.7392	1.4352	1.0059	0.1543
754.04	0.0576	0.0506	38.1620	1.5472	1.0009	0.1891
757.20	0.0207	0.0190	14.4095	1.6296	0.9993	0.2123

PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t
1	702.2685	7.6110	92.2697
2	-798.0359	40.5974	-19.6573
3	865.1155	67.6878	12.7810
4	-340.7344	35.3320	-9.6438

Degrees of Freedom= 12
Confidence In First Term= 99.5%+
Confidence In Last Term= 99.5%+

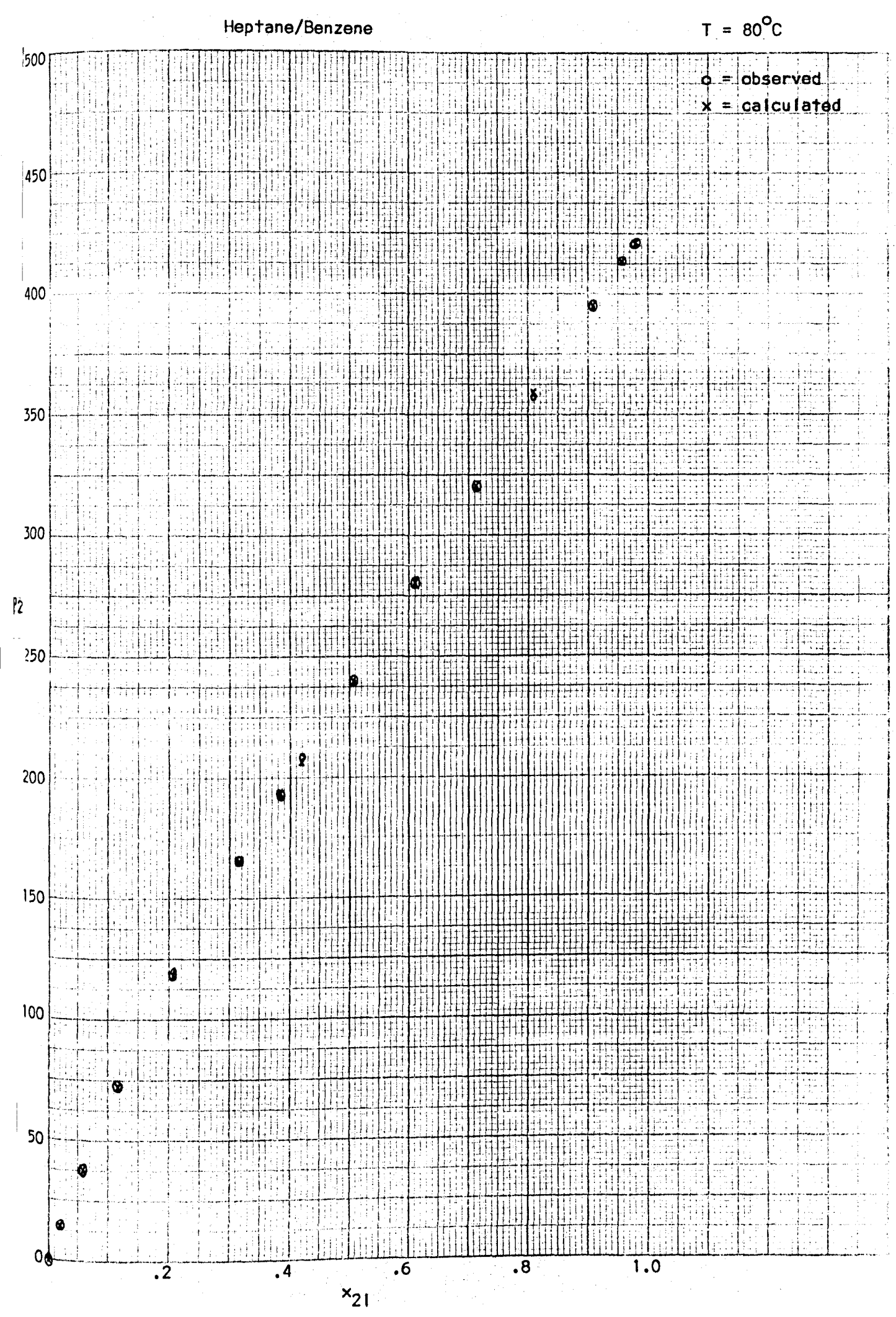
P_2 CALC.	DIF.
421.3532	-0.0864
413.1444	0.1089
412.6335	-0.3852
395.4096	0.8635
358.5346	-0.9620
320.0115	0.7068
280.2792	-0.3842
240.3247	-0.1256
206.9246	1.3637
193.6359	-0.7587
165.8017	-0.8976
118.6271	1.0137
72.4475	-0.7083
37.9831	0.1789
14.1758	0.2337

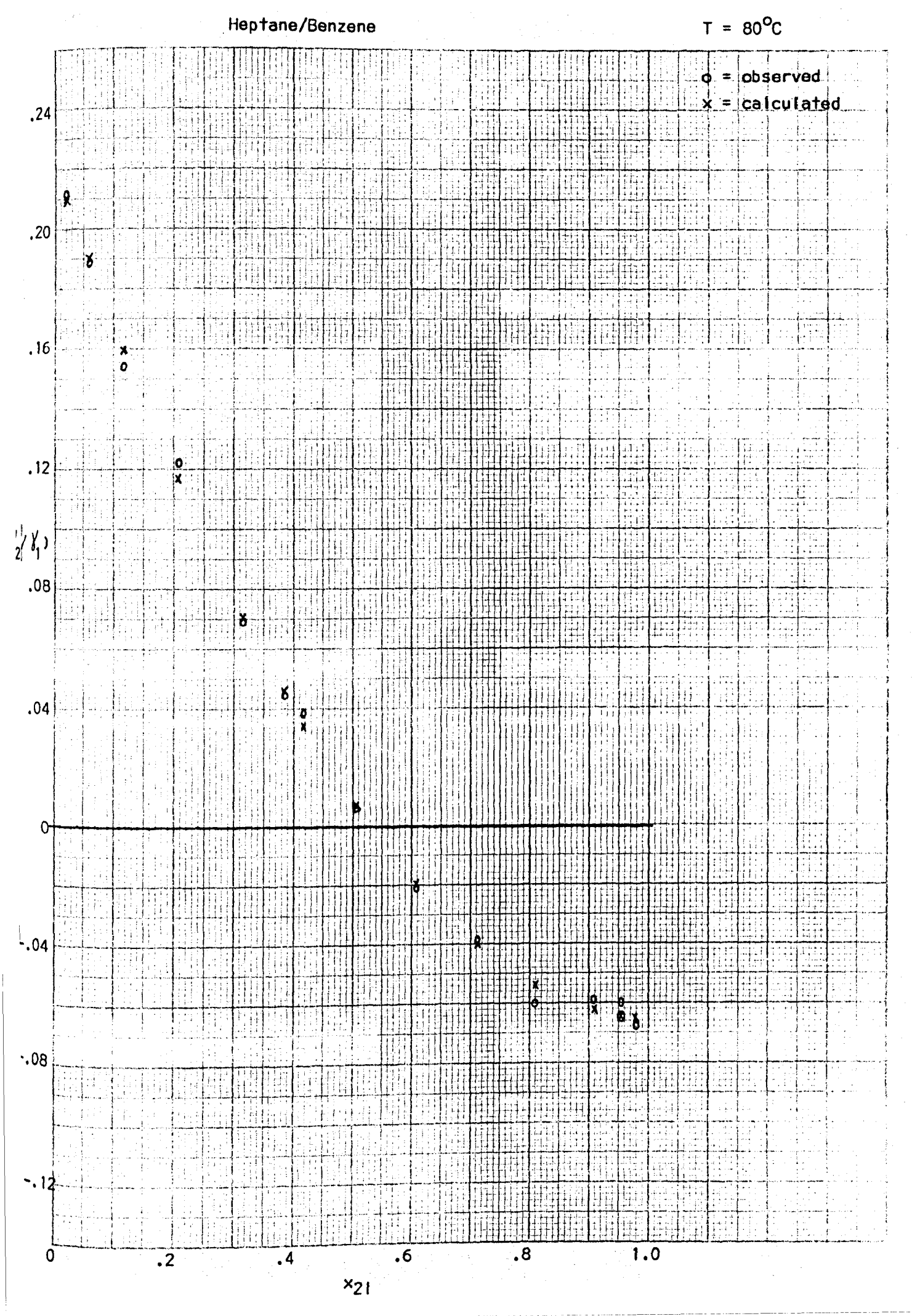
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t
0	0.2220	0.0026	84.7498
1	-0.5667	0.0124	-45.7340
2	0.2789	0.0116	24.1479

Degrees of Freedom= 12
Integral at x=1: 0.0316
Error in Integral: 0.0034

$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
-0.0655	-0.0028
-0.0648	0.0047
-0.0648	-0.0008
-0.0625	0.0031
-0.0541	-0.0058
-0.0400	0.0013
-0.0197	-0.0018
0.0070	-0.0007
0.0339	0.0049
0.0455	-0.0013
0.0711	-0.0018
0.1163	0.0057
0.1597	-0.0053
0.1903	-0.0012
0.2105	0.0019


Heptane/Benzene
T = 80°C
o = observed
x = calculated
500
450
400
350
300
P2
250
200
150
100
50
0
.2
.4
.6
.8
1.0
x21


Heptane/Benzene
T = 80°C
o = observed
x = calculated
.24
.20
.16
.12
.08
.04
0
-.04
-.08
-.12
0
.2
.4
.6
.8
1.0
x21

System: Toluene/Benzene T= 120°C.

Reference: Griswold,Andres ,Klein(1943):Physico-Chemical Constants of Binary Systems,Timmerman

p_{12}	x_{21}	x_{2v}	p_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
1132.40	0.8830	0.7800	883.2720	1.0334	0.9430	0.0397
1322.40	0.7440	0.5780	764.3472	1.0613	0.9654	0.0411
1330.00	0.7420	0.5750	764.7500	1.0647	0.9703	0.0403
1322.40	0.7360	0.4470	791.1128	0.8297	1.2268	-0.1698
1520.00	0.5600	0.3610	548.7200	1.0122	0.9776	0.0151
1869.60	0.3120	0.1760	329.0496	1.0895	0.9917	0.0409

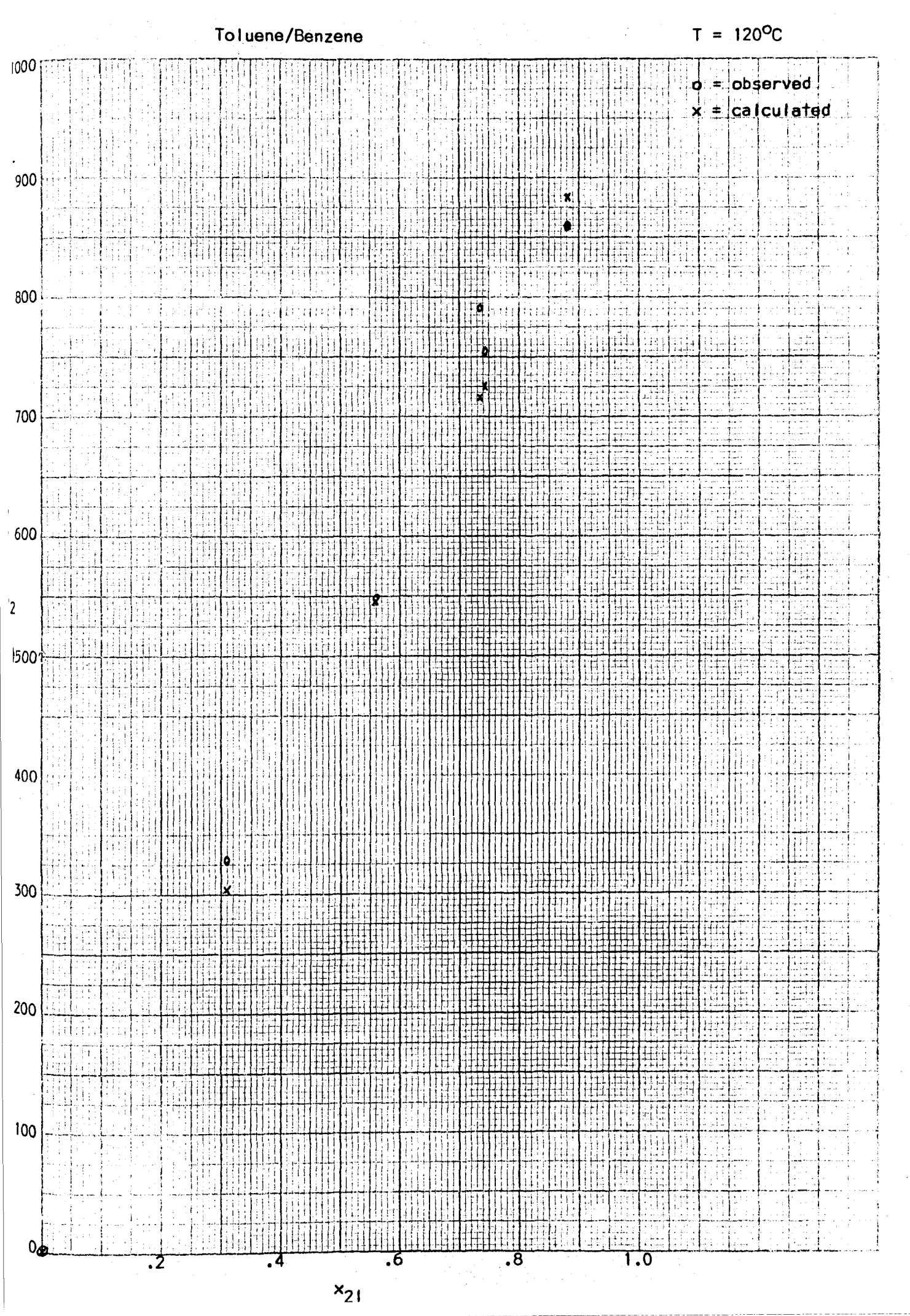
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	973.4260	34.5702	28.1580	859.5351	23.7369
				724.2289	40.1183
Degrees of Freedom= 6				722.2821	42.4679
Confidence in First Term= 99.5%+				716.4415	-125.3287
				545.1186	3.6014
				303.7089	25.3407

THERMODYNAMIC CONSISTENCY CURVE FITTING:

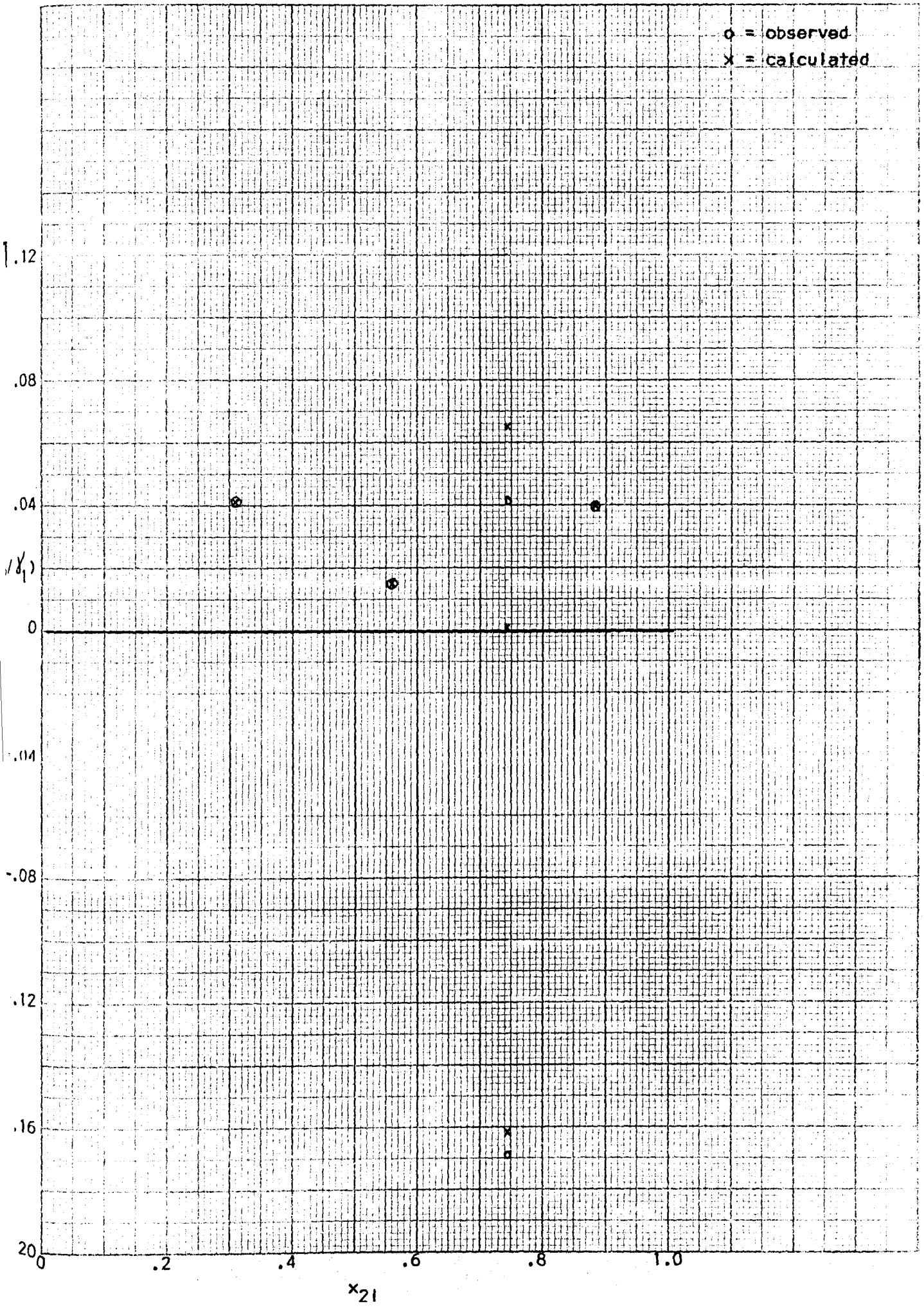
n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	-294.7496	72.3956	-4.0714	0.0397	0.0000
1	2202.4308	541.0088	4.0710	0.0652	-0.0241
2	-5786.1035	1421.8593	-4.0694	0.0082	0.0322
3	6429.3861	1580.8320	4.0671	-0.1617	-0.0081
4	-2574.3826	633.4050	-4.0644	0.0151	0.0000
				0.0409	0.0000

Degrees of Freedom= 1
Integral at x=1: -29.7654
Error in Integral: 0.0168


Toluene/Benzene
T = 120°C
o = observed
x = calculated
1000
900
800
700
600
1500
400
300
200
100
0
.2
.4
.6
.8
1.0
x_{21}

Toluene/Benzene

T = 120°C



System: Toluene/Benzene T= 160°C.

Reference: Griswold,Andres,Klein(1943):Physico-Chemical Constants of Binary Systems,Timmerman

p_{12}	x_{21}	x_{2v}	p_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
2872.80	0.8730	0.7720	2217.8016	1.0412	0.9226	0.0525
3275.60	0.7230	0.5860	1919.5016	1.0881	0.8758	0.0942
3594.80	0.6020	0.4570	1642.8236	1.1184	0.8774	0.1054
4263.60	0.3800	0.2480	1057.3728	1.1404	0.9251	0.0908
4871.60	0.2400	0.1550	755.0980	1.2894	0.9690	0.1241

PARTIAL PRESSURE CURVE FITTING:

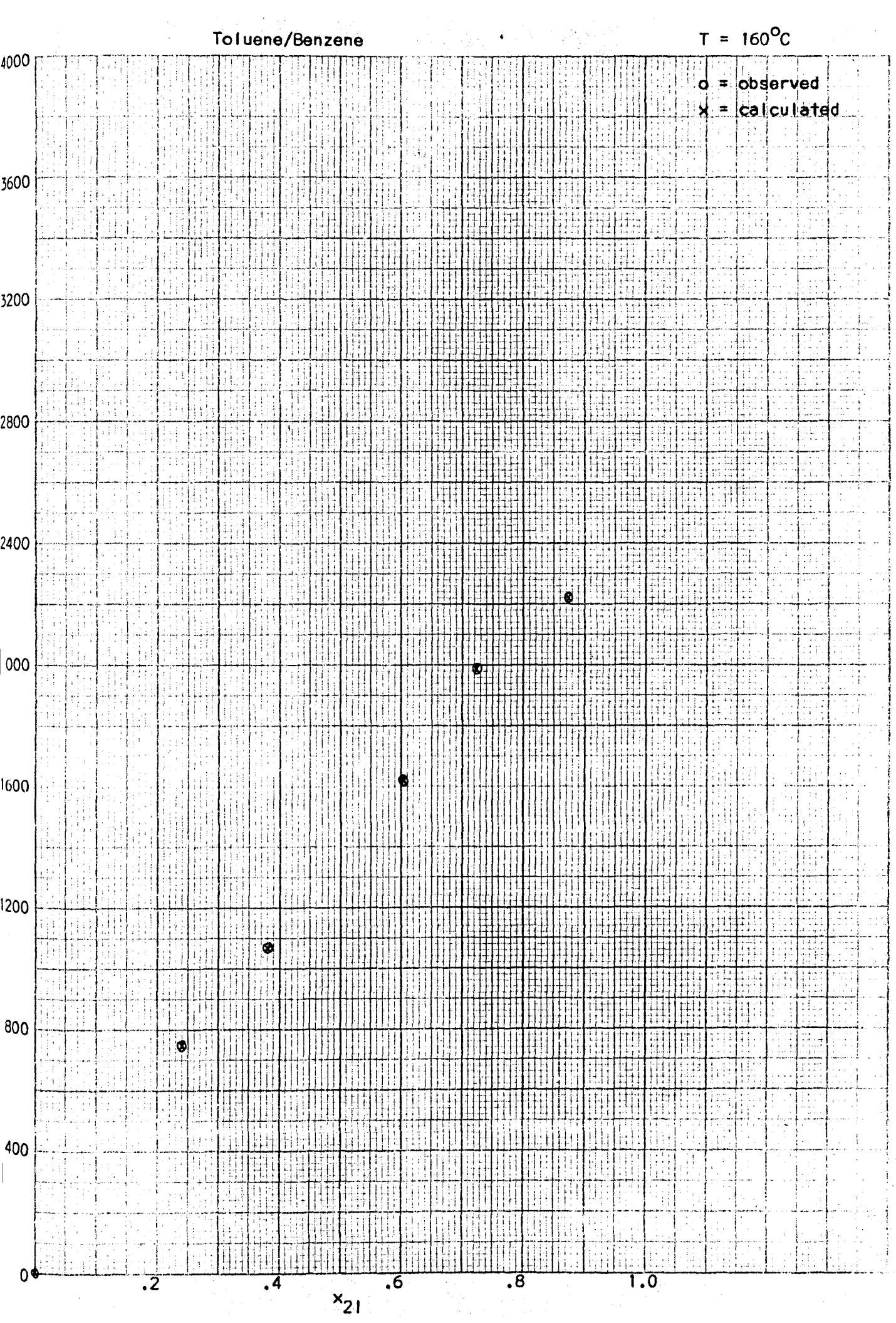
n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	4399.5864	505.2522	8.7077	2215.2573	2.5443
2	-8043.7431	2942.9274	-2.7332	1932.4627	-12.9611
3	12890.4431	5223.9056	2.4676	1625.0619	17.7617
4	-7010.0494	2892.9159	-2.4232	1071.4817	-14.1089
				747.5210	7.5770

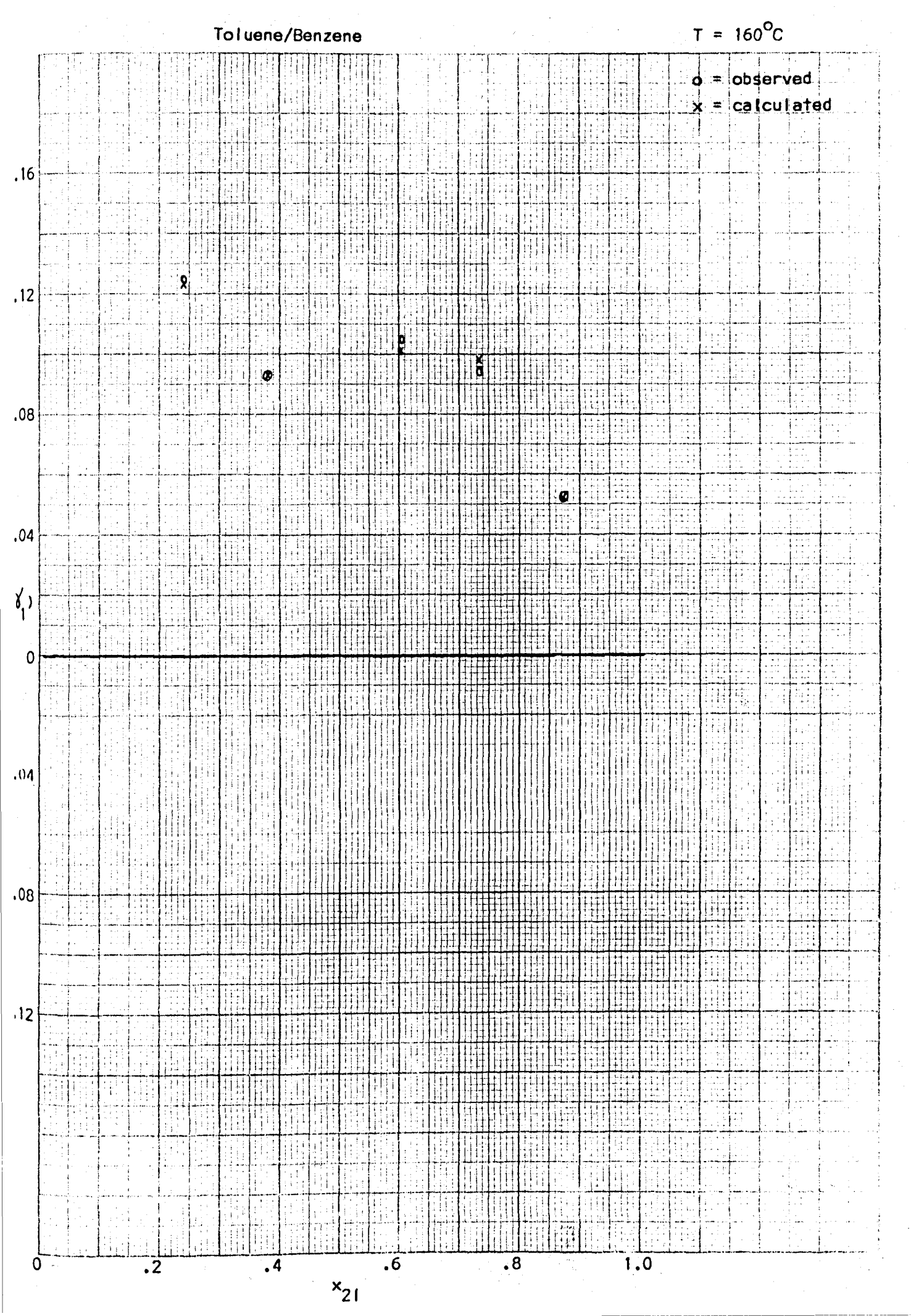
Degrees of Freedom= 2
Confidence in First Term= 99.0%+
Confidence in Last Term= 90.0%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.3373	0.0587	5.7429	0.0516	0.0009
1	-1.4818	0.3763	-3.9381	0.0981	-0.0039
2	2.8913	0.7165	4.0353	0.1010	0.0044
3	-1.7970	0.4203	-4.2758	0.0931	-0.0022
				0.1233	0.0008

Degrees of Freedom= 1
Integral at x=1: 0.1109
Error in Integral: 0.0029


Toluene/Benzene
T = 160°C
o = observed
x = calculated
4000
3600
3200
2800
2400
000
1600
1200
800
400
0
.2
.4
.6
.8
1.0
x21


Toluene/Benzene
T = 160°C
o = observed
x = calculated
.16
.12
.08
.04
γ_1
0
.04
.08
.12
0
.2
.4
.6
.8
1.0
x_{21}

System: Toluene/Benzene T= 200°C.

Reference: Griswold,Andres,Klein(1943):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
6771.60	0.8460	0.7780	5268.3048	1.0077	0.9270	0.0362
7235.20	0.7300	0.6160	4456.8832	0.9879	0.9772	0.0047
7911.60	0.6150	0.4820	3813.3912	1.0033	1.0109	-0.0033
8686.80	0.4340	0.3180	2762.4024	1.0299	0.9940	0.0154
9720.40	0.2230	0.1540	1496.9416	1.0862	1.0051	0.0337

PARTIAL PRESSURE CURVE FITTING:

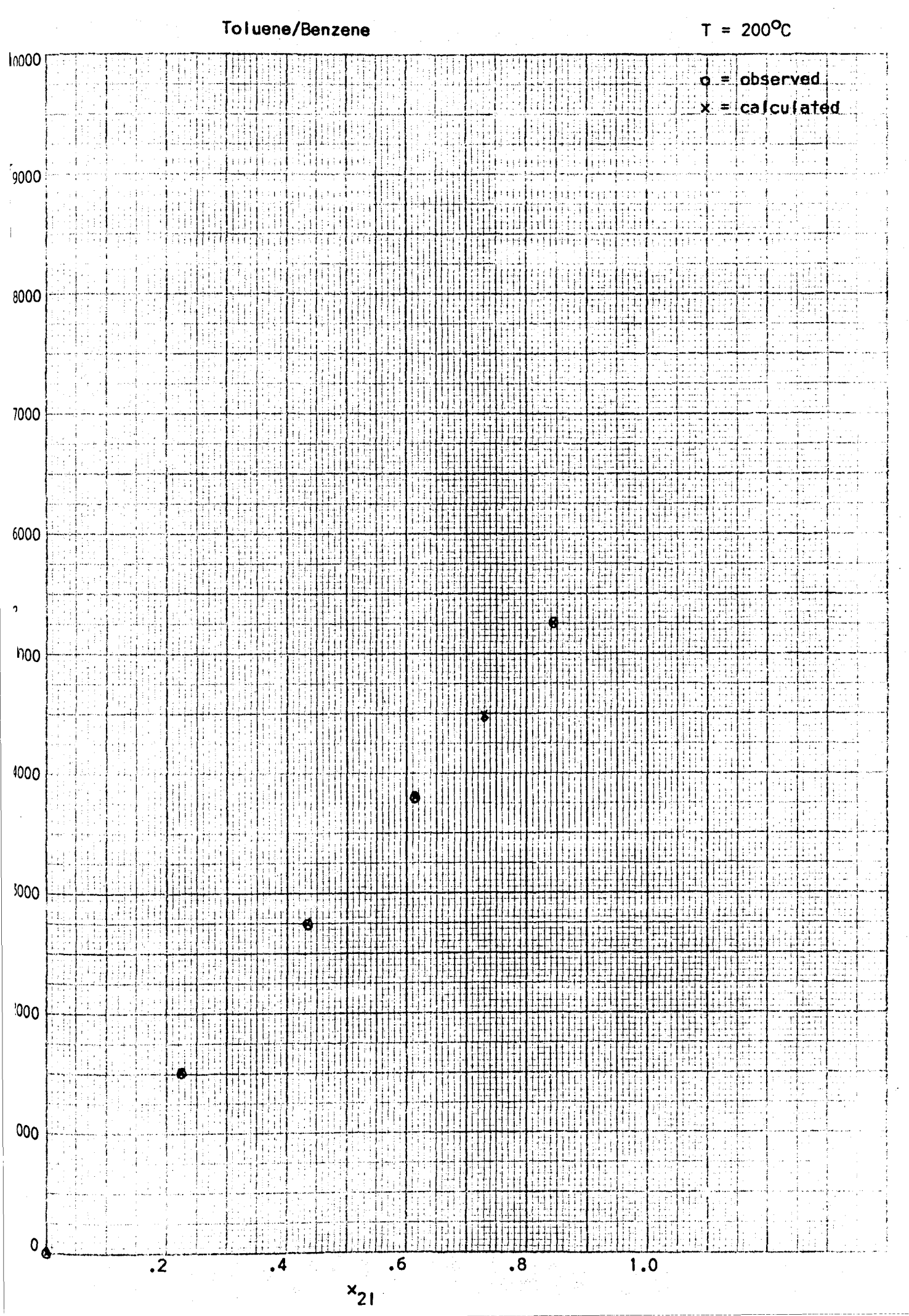
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	7488.1055	242.6145	30.8642	5254.6781	13.6267
2	-3839.3115	806.6001	-4.7599	4491.7407	-34.8575
3	2754.1029	647.1750	4.2556	3793.6887	19.7025
				2751.8187	10.5837
				1509.4642	-12.5226

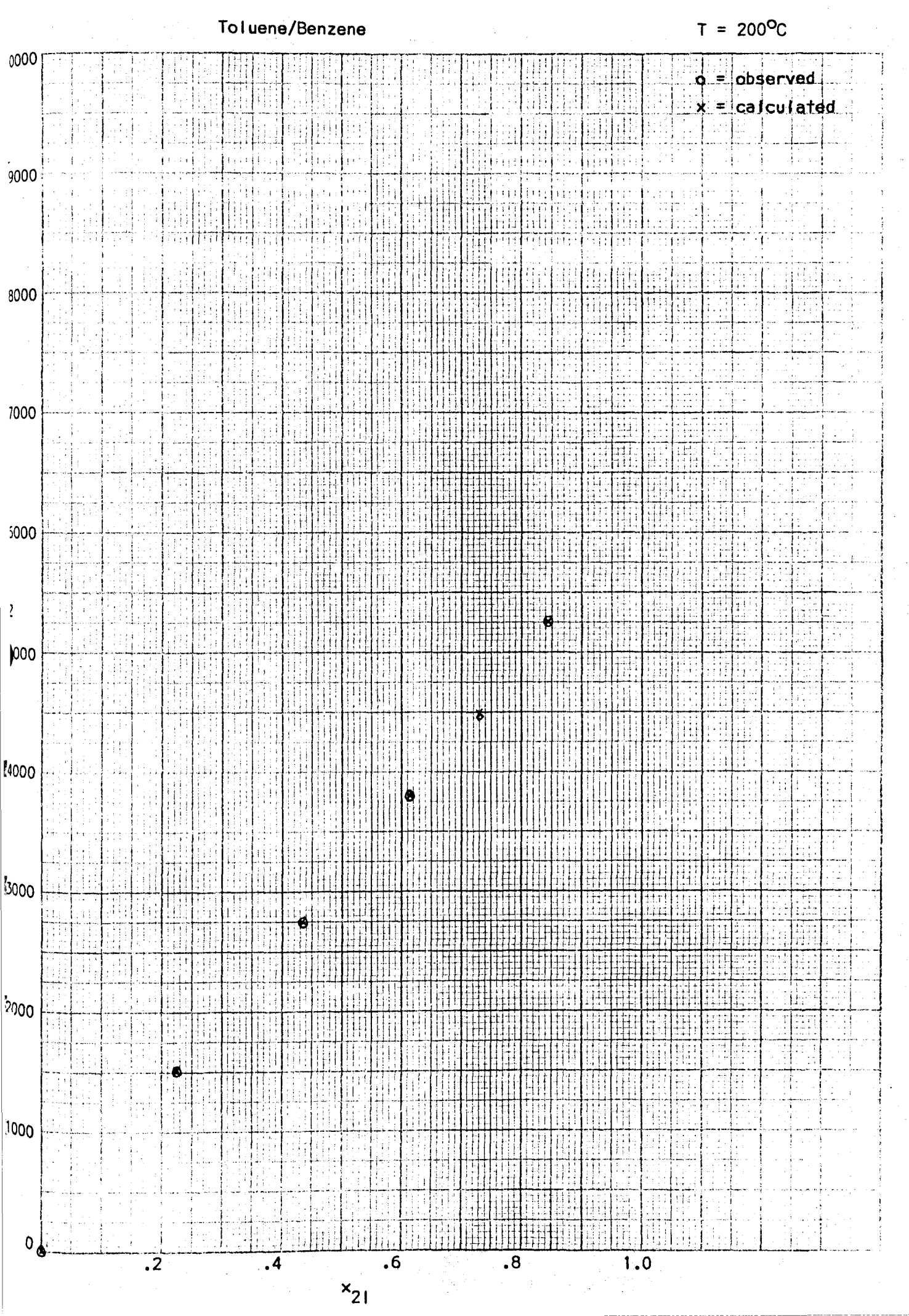
Degrees of Freedom= 3
Confidence in First Term= 99.5%+
Confidence in Last Term= 97.5%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1043	0.0304	3.4319	0.0307	0.0055
1	-0.3772	0.1273	-2.9626	0.0117	-0.0070
2	0.3430	0.1182	2.9-24	0.0020	-0.0053
				0.0052	0.0102
				0.0372	-0.0035

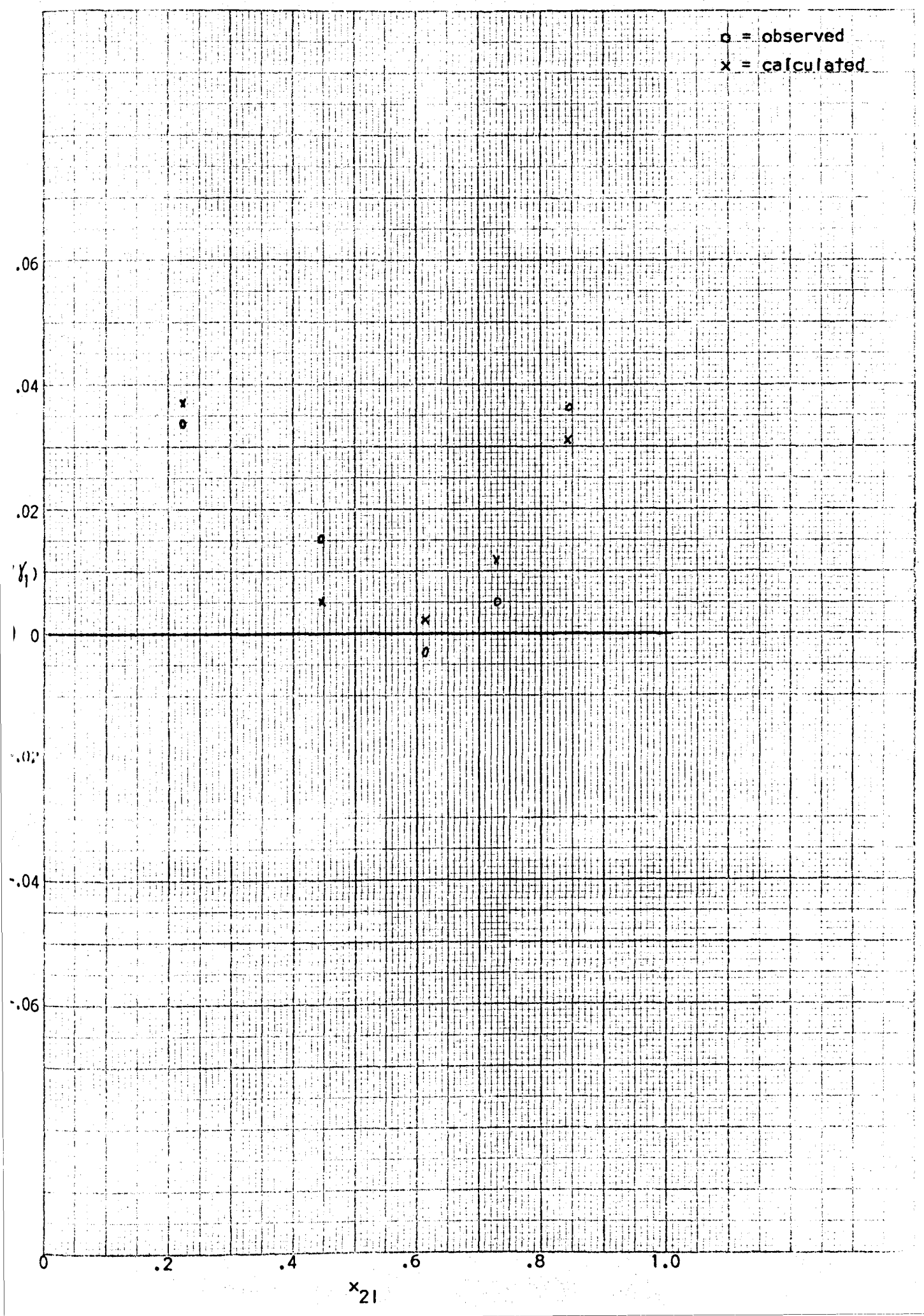
Detrees of Freedom= 2
Integral at x=1: 0.0300
Error in Integral: 0.0067


Toluene/Benzene
T = 200°C
o = observed
x = calculated
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
.2
.4
.6
.8
1.0
x_{21}


Toluene/Benzene
T = 200°C
o = observed
x = calculated
0000
9000
8000
7000
5000
000
4000
3000
2000
1000
0
.2
.4
.6
.8
1.0
x21

Toluene/Benzene

T = 200°C



System: Toluene/Benzene T= 240°C.

Reference: Griswold,Andres,Klein(1943):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
12312.00	0.8290	0.7630	9394.0560	1.0600	0.9199	0.0616
13604.00	0.6920	0.5830	7931.1320	1.0721	0.9929	0.0333
15481.20	0.4930	0.3920	6068.6304	1.1515	1.0008	0.0609
15982.80	0.4500	0.3340	5338.2552	1.1097	1.0433	0.0268
17328.00	0.2410	0.1710	2963.0880	1.1501	1.0203	0.0520

PARTIAL PRESSURE CURVE FITTING:

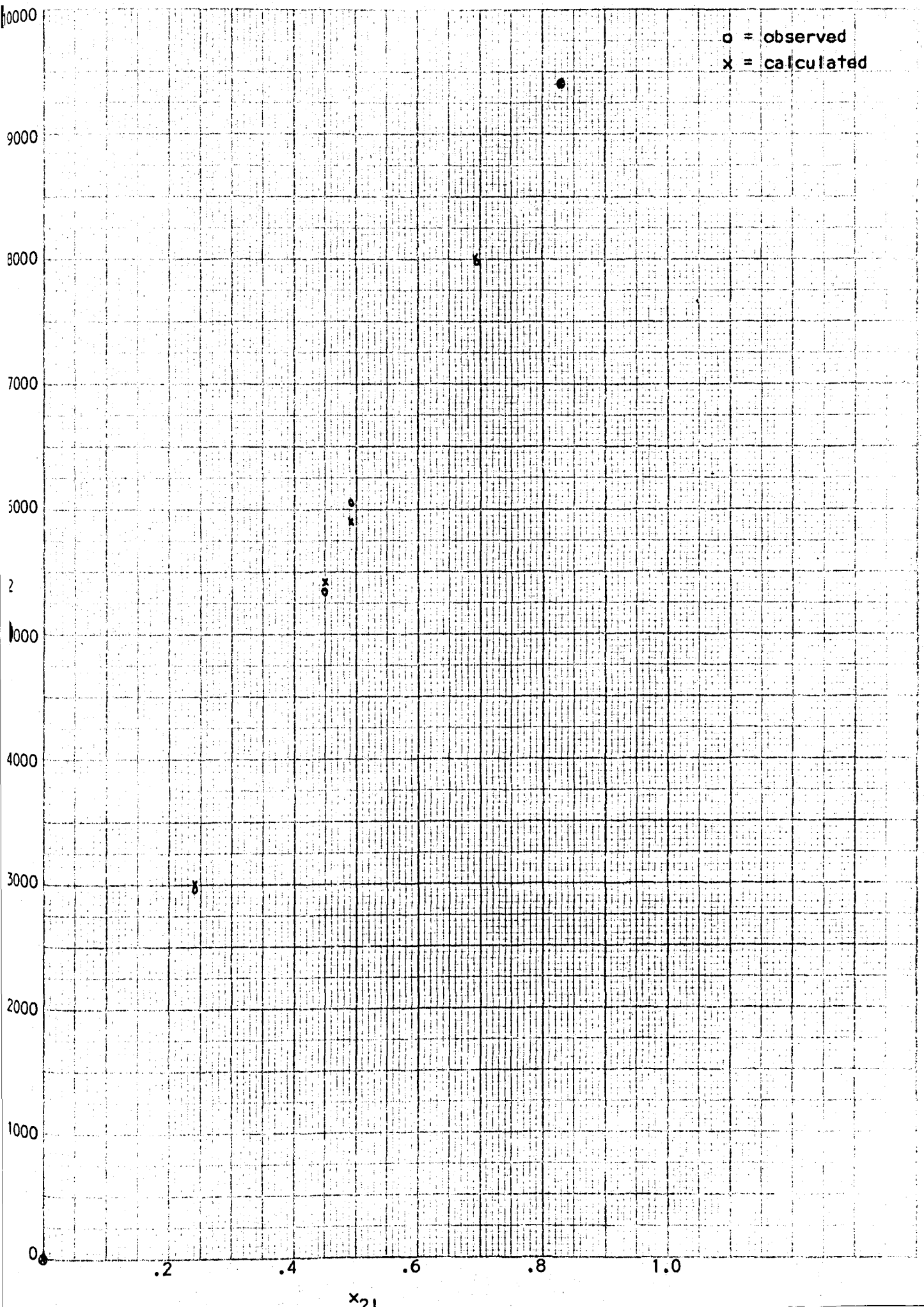
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	12943.5735	341.0962	37.9370	9370.3371	23.7189
2	-1978.7604	491.2309	-4.0282	8009.3957	-78.2637
				5900.2460	168.3844
Degrees of Freedom=.4				5423.9091	-85.6539
Confidence in First Term= 99.5%+				3004.4728	-41.3848
Confidence in Last Term= 99.0%+					

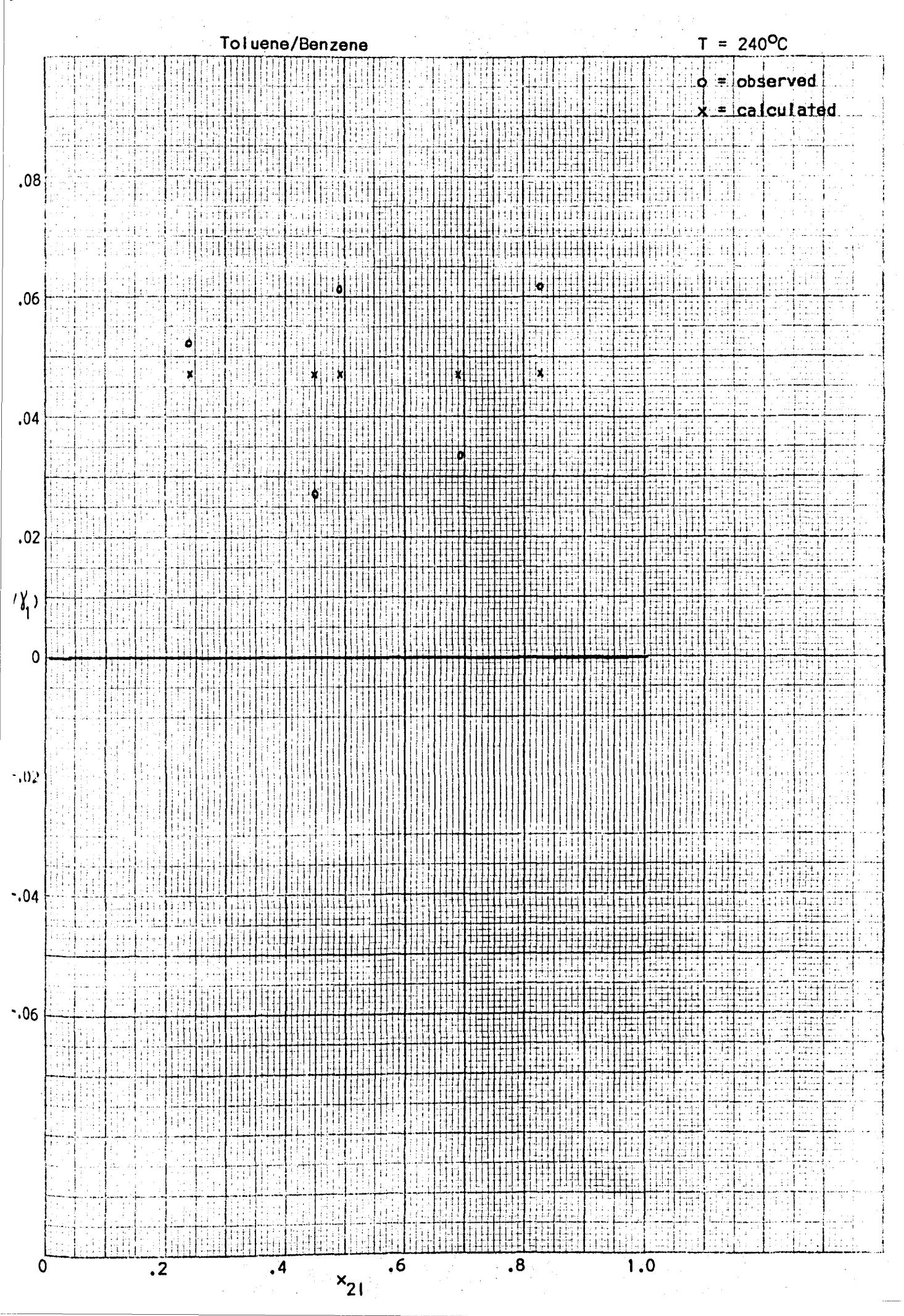
THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.0469	0.0072	6.5510	0.0469	0.0146
				0.0469	-0.0136
Degrees of Freedom= 4				0.0469	0.0140
Integral at x=1: 0.0469				0.0469	-0.0201
Error in Integral: 0.0143				0.0469	0.0051

Toluene/Benzene

T = 240°C




Toluene/Benzene
T = 240°C
o = observed
x = calculated
.08
.06
.04
.02
(γ_1)
0
-.02
-.04
-.06
0
.2
.4
.6
.8
1.0
x_{21}

System: Toluene/Benzene T= 280°C.

Reference: Griswold,Andres,Klein(1943):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
21257.20	0.8310	0.7880	16750.6736	1.0866	0.8068	0.1293
23172.40	0.6980	0.6220	14413.2328	1.1132	0.8776	0.1033
23636.00	0.6450	0.5730	13543.4280	1.1319	0.8602	0.1192
25893.20	0.4300	0.3560	9217.9792	1.1556	0.8852	0.1158
28963.60	0.2570	0.2100	6082.3560	1.2758	0.9318	0.1365

PARTIAL PRESSURE CURVE FITTING:

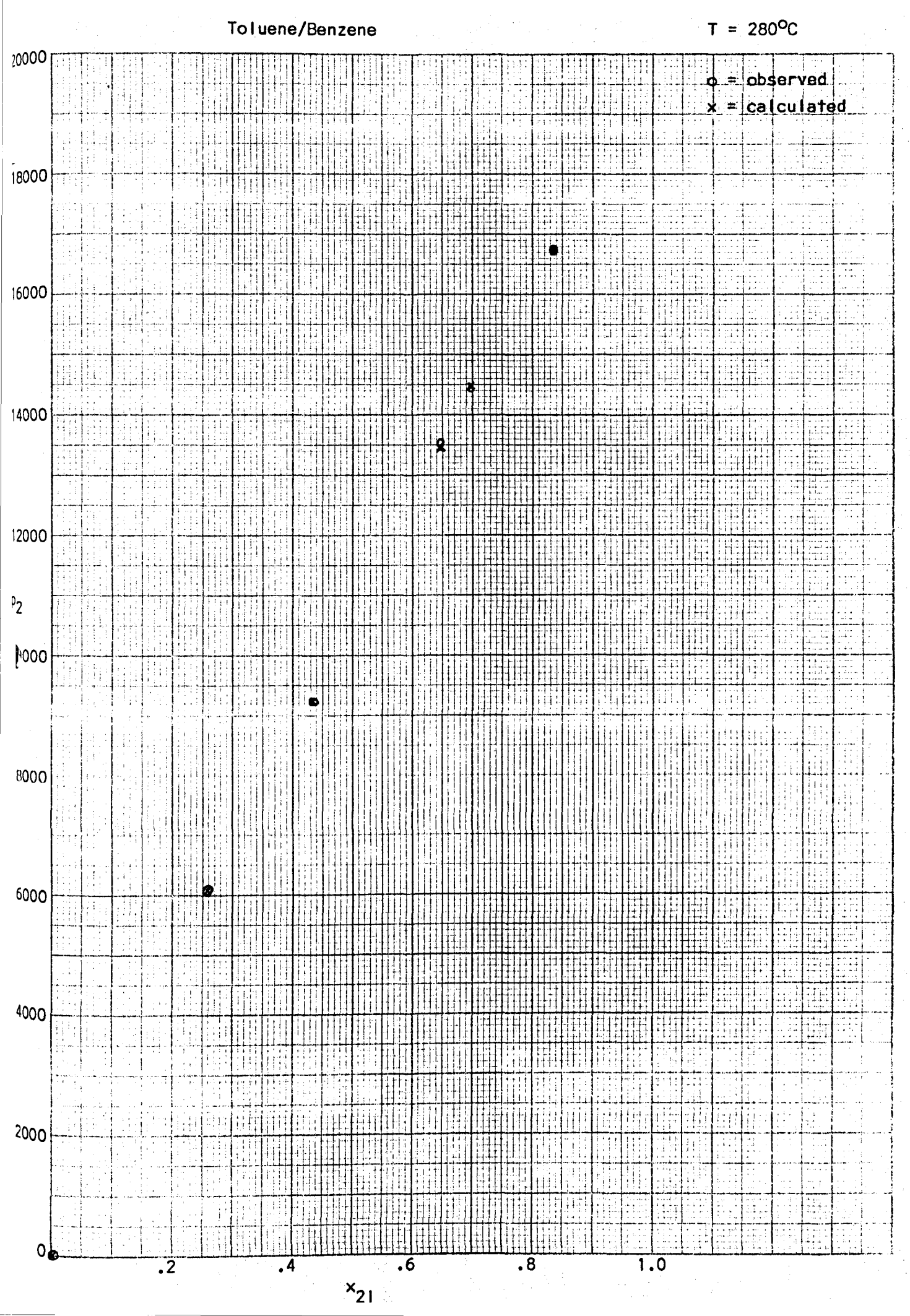
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	32717.3979	2580.9236	12.6766	16741.0141	9.6595
2	-54240.6186	15061.7797	-3.6012	14491.8323	-78.5995
3	85200.8612	27125.9774	3.1409	13457.2578	86.1702
4	-45889.9137	15392.1284	-2.9814	9244.5708	-26.5916
				6071.8892	10.4668

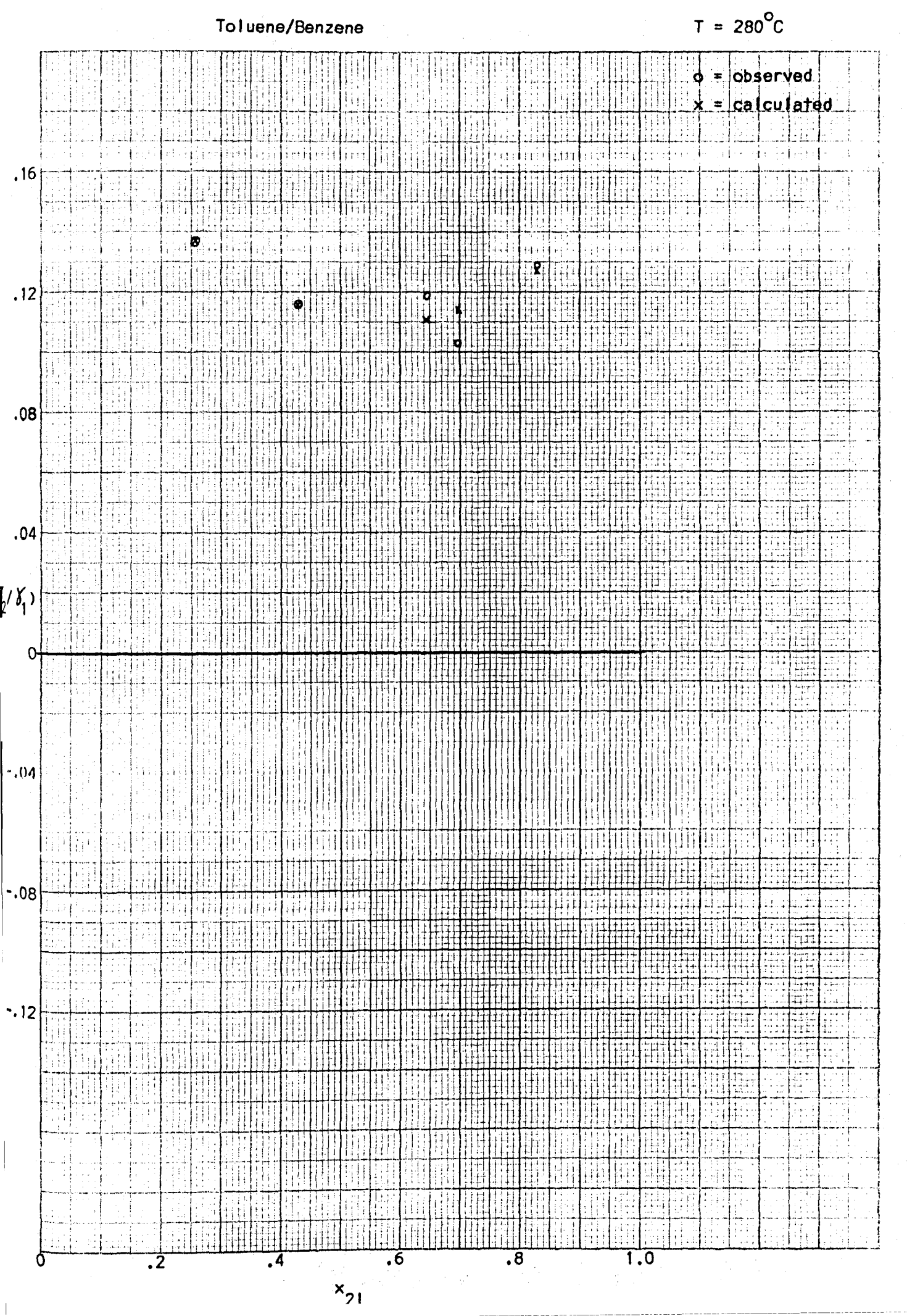
Degrees of Freedom= 2
Confidence in First Term= 99.5%+
Confidence in Last Term= 95.0%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.1980	0.0343	5.7730	0.1269	0.0024
1	-0.3058	0.1407	-2.1726	0.1137	-0.0104
2	0.2650	0.1295	2.0465	0.1110	0.0082
				0.1155	0.0003
				0.1369	-0.0004

Degrees of Freedom= 2
Integral at x=1: 0.1334
Error in Integral: 0.0060


Toluene/Benzene
T = 280°C
o = observed
x = calculated
20000
18000
16000
14000
12000
p_2
8000
6000
4000
2000
0
.2
.4
.6
.8
1.0
x_{21}


Toluene/Benzene
T = 280°C
o = observed
x = calculated
.16
.12
.08
.04
0
-.04
-.08
-.12
0
.2
.4
.6
.8
1.0
x_{21}

System: Tetraethylsilane/Benzene T= 20°C.

Reference: Bjerrum,Jozefowicz(1932):Physico-Chemical Constants of Binary Systems,Timmerman

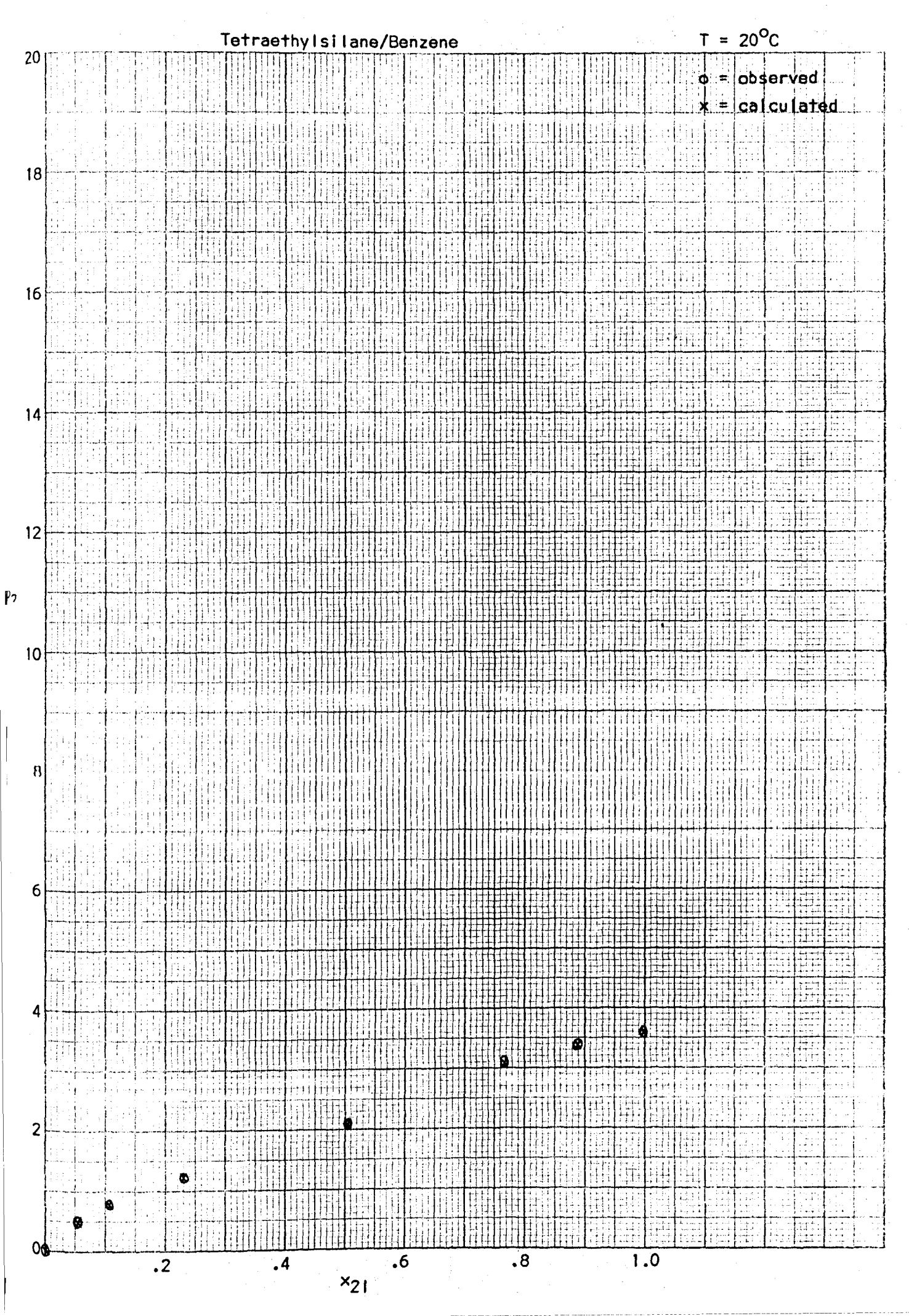
p_{12}	x_{21}	x_{2v}	p_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
75.81	0.0000	0.0000	0.0000	1.0000	1.0000	------
73.28	0.0549	0.0060	0.4397	2.1882	1.0166	0.3329
70.03	0.1078	0.0114	0.7983	2.0234	1.0236	0.2960
63.38	0.2310	0.0192	1.2227	1.4461	1.0713	0.1303
47.81	0.5025	0.0435	2.0797	1.1308	1.2125	-0.0303
27.66	0.7671	0.1109	3.0675	1.0926	1.3929	-0.1055
16.18	0.8896	0.2074	3.3557	1.0307	1.5323	-0.1722
3.66	1.0000	1.0000	3.6600	1.0000	1.0000	------

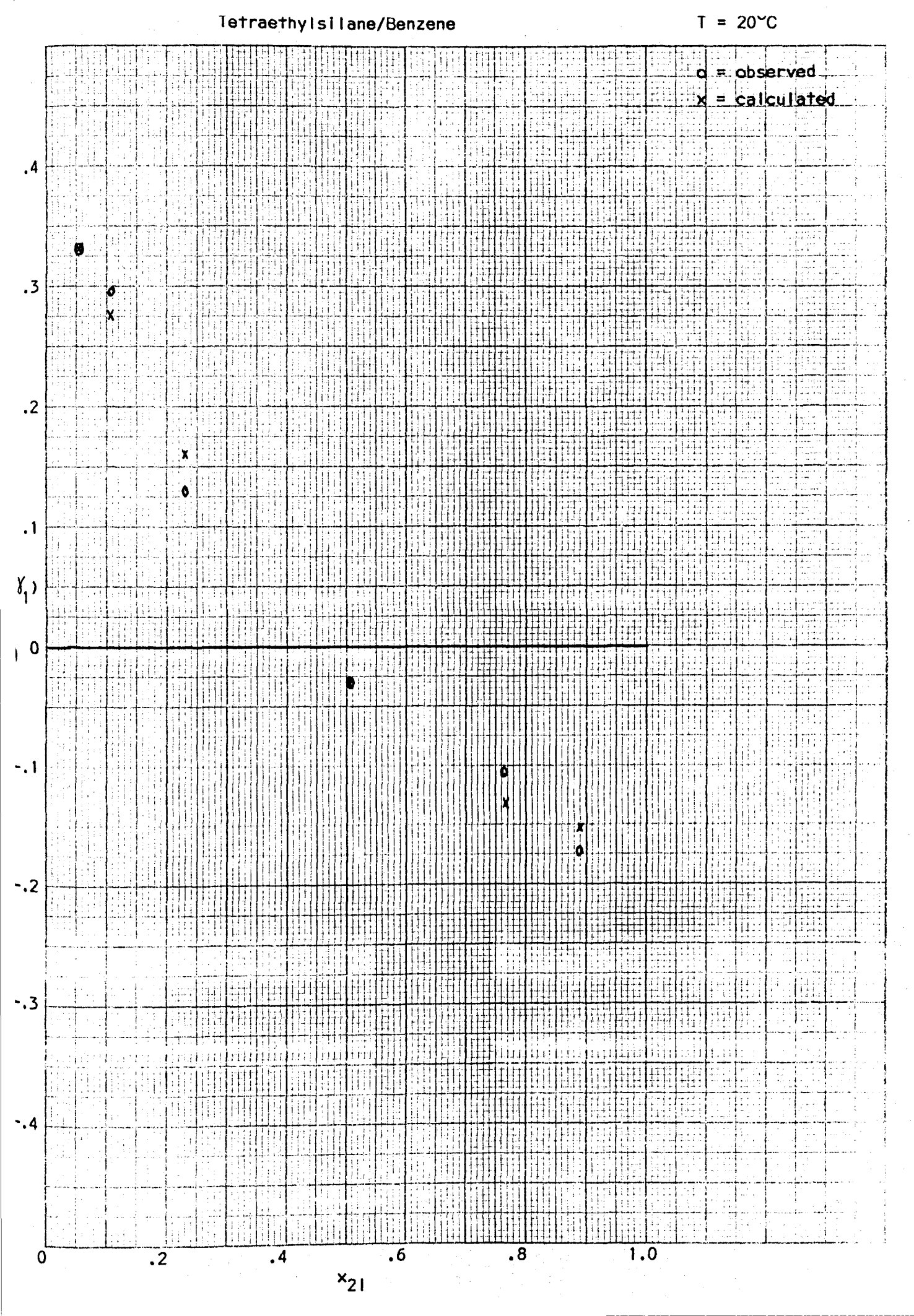
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	10.4216	0.4754	21.9223	0.0000	0.0000
2	-37.6989	4.4478	-8.4758	0.4717	-0.0320
3	84.0223	13.2693	6.3321	0.7800	0.0183
4	-81.6263	15.6319	-5.2218	1.2178	0.0049
5	28.5380	6.3499	4.4942	2.0886	-0.0089
				3.0539	0.0136
Degrees of Freedom= 3				3.3677	-0.0120
Confidence in First Term=99.5%+				3.6567	0.0033
Confidence in Last Term= 99.0%+					

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.3932	0.0288	13.6747	------	------
1	-1.1463	0.1778	-6.4463	0.3321	0.0008
2	0.5990	0.1866	3.2091	0.2766	0.0194
				0.1604	-0.0301
Degrees of Freedom= 3				-0.0316	0.0013
Integral at x=1: 0.0197				-0.1337	0.0282
Error in Integral: 0.0203				-0.1526	-0.0197
				-------	------


Tetraethylsilane/Benzene
T = 20°C
o = observed
x = calculated
20
18
16
14
12
10
8
6
4
2
0
.2
.4
.6
.8
1.0
x21


Tetraethylsilane/Benzene
T = 20°C
o = observed
x = calculated
.4
.3
.2
.1
γ_1
0
-.1
-.2
-.3
-.4
0
.2
.4
.6
.8
1.0
x_{21}

System: Tetraethylsilane/Benzene T= 35°C.

Reference: Bjerrum,Jozefowicz(1932):Physico-Chemical Constants of Binary Systems,Timmerman

p_{12}	x_{21}	x_{2v}	p_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
150.80	0.0000	0.0000	0.0000	1.0000	1.0000	------
144.30	0.0536	0.0060	0.8658	1.8567	1.0050	0.2666
142.40	0.0760	0.0086	1.2246	1.8521	1.0132	0.2620
122.50	0.2550	0.0247	3.0257	1.3639	1.0634	0.1081
92.30	0.5008	0.0539	4.9750	1.1418	1.1600	-0.0069
54.50	0.7853	0.1236	6.7362	1.0211	1.3105	-0.1084
28.20	0.9179	0.2842	8.0144	1.0036	1.6304	-0.2107
8.70	1.0000	1.0000	8.7000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

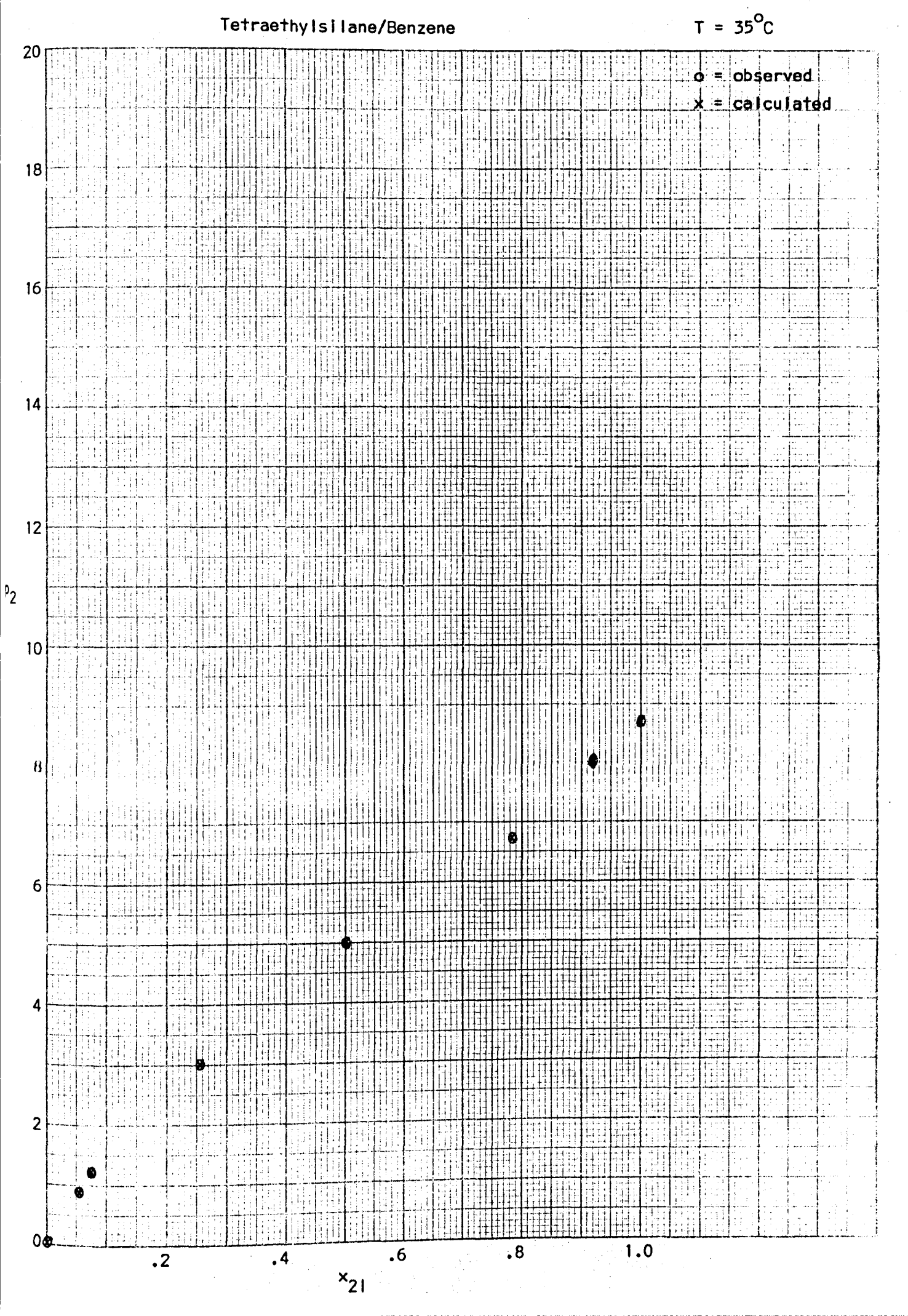
n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	19.1926	0.5986	32.0636	0.0000	0.0000
2	-55.0700	7.2875	-7.5568	0.8923	-0.0265
3	154.2746	31.8122	4.8495	1.2006	0.0241
4	-245.5348	62.6988	-3.9161	3.0287	-0.0029
5	197.0071	57.0010	3.4562	4.9737	0.0013
6	-61.1694	19.4323	-3.1478	6.7371	-0.0009
				8.0138	0.0007
				8.7003	-0.0003

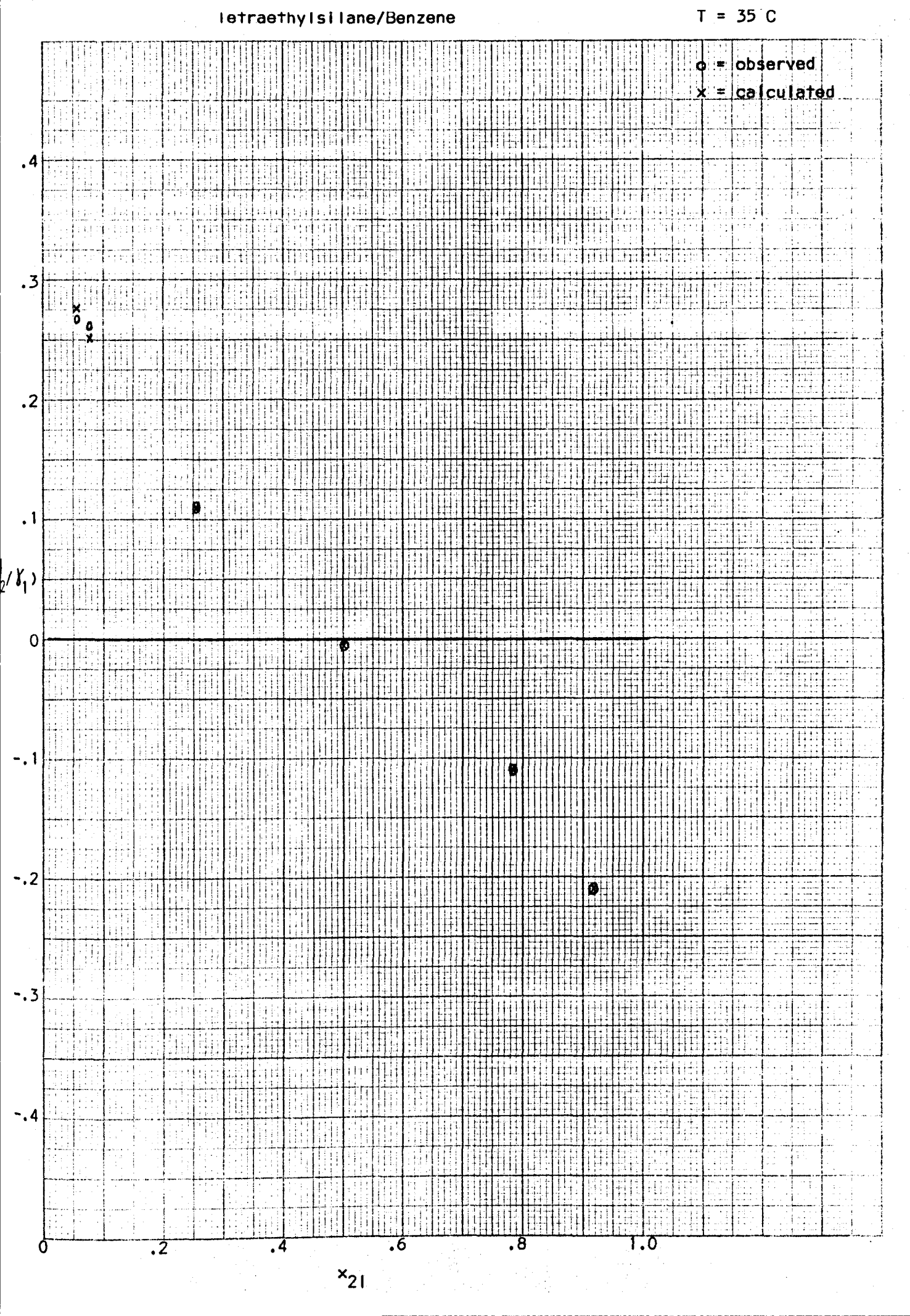
Degrees of Freedom= 2
Confidence in First Term= 99.5%+
Confidence in Last Term= 95.0%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.3372	0.0125	26.9388	------	------
1	-1.2379	0.1456	-8.5017	0.2753	-0.0087
2	1.5932	0.3705	4.3003	0.2519	0.0101
3	-0.9741	0.2544	-3.8293	0.1090	-0.0009
				-0.0055	-0.0014
				-0.0101	0.0017
				0.2100	-0.0007
				------	------

Degrees of Freedom= 2
Integral at x=1: 0.0058
Error in Integral; 0.0055


Tetraethylsilane/Benzene
T = 35°C
o = observed
x = calculated
20
18
16
14
12
10
8
6
4
2
0
p_2
.2
.4
.6
.8
1.0
x_{21}


Tetraethylsilane/Benzene
T = 35 C
o = observed
x = calculated
.4
.3
.2
.1
0
-.1
-.2
-.3
-.4
0
.2
.4
.6
.8
1.0
x_{21}

System: Tetraethylsilane/Benzene T= 50°C.

Reference: Bjerrum,Jozefowicz(1932):Physico-Chemical Constants of Binary Systems,Timmerman

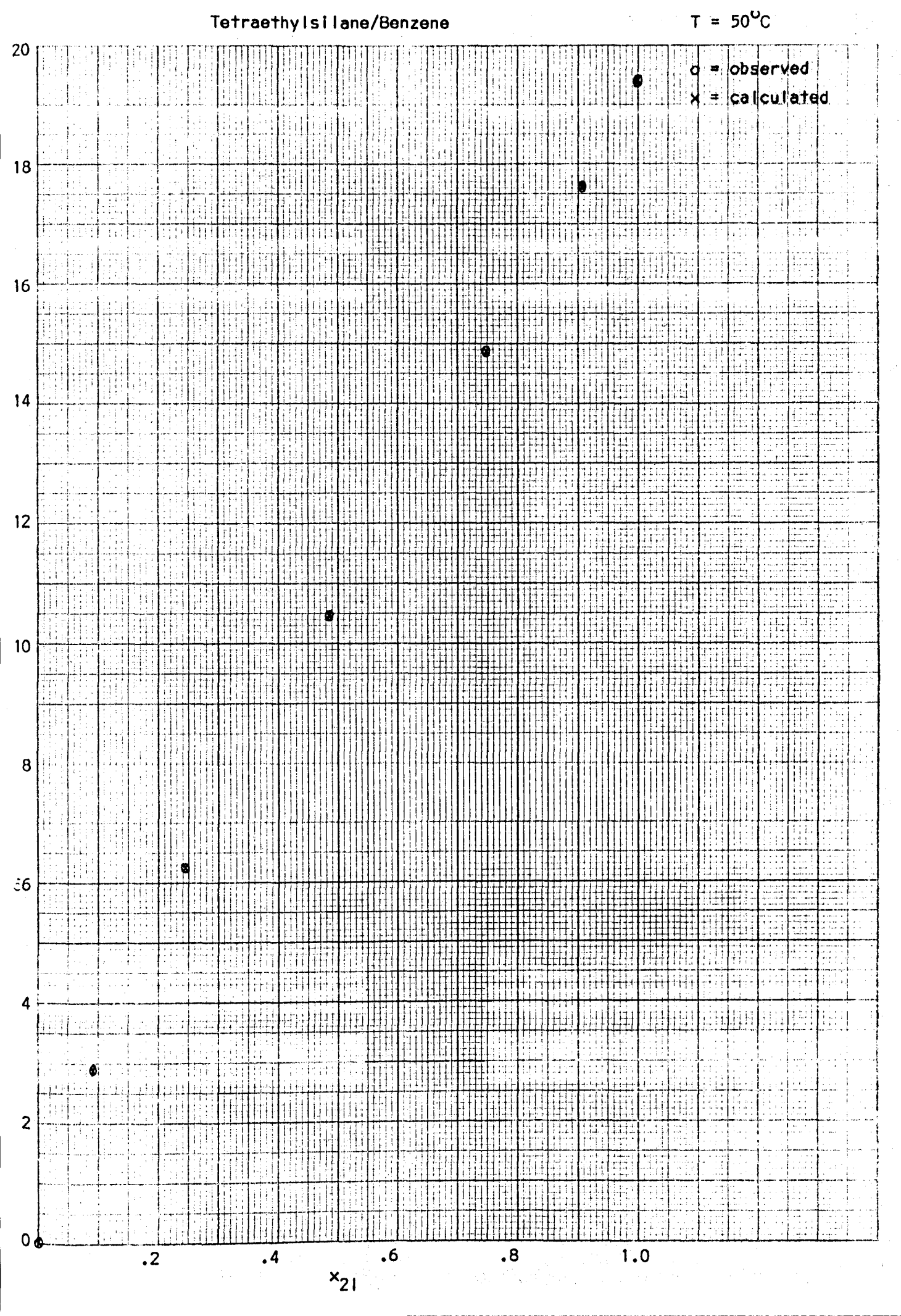
p_{12}	x_{21}	x_{2v}	p_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
276.30	0.0000	0.0000	0.0000	1.0000	1.0000	------
255.40	0.0939	0.0113	2.8860	1.5818	1.0086	0.1954
223.80	0.2448	0.0280	6.2664	1.3174	1.0425	0.1017
168.70	0.4874	0.0619	10.4425	1.1027	1.1174	-0.0058
102.00	0.7493	0.1458	14.8716	1.0215	1.2578	-0.0904
54.70	0.9064	0.3220	17.6134	1.0001	1.4340	-0.1565
19.43	1.0000	1.0000	19.4300	1.0000	1.0000	-------

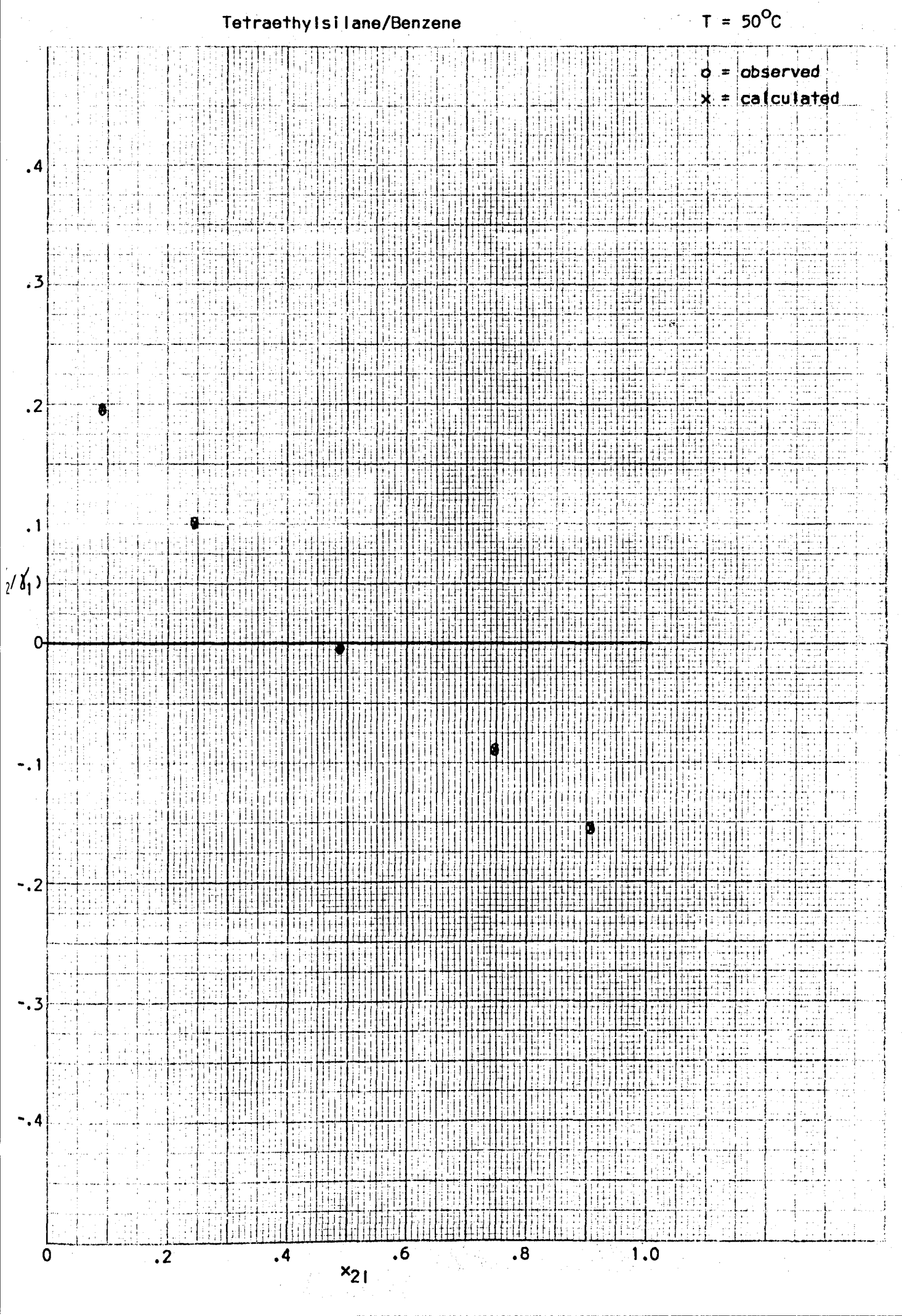
PARTIAL PRESSURE CURVE FITTING:

n	a_n	STD.ERROR	t	p_2 CALC.	DIF.
1	35.8922	0.4398	81.6174	0.0000	0.0000
2	-62.2319	3.7683	-16.5146	2.8978	-0.0118
3	99.2086	10.7954	9.1899	6.2524	0.0140
4	-78.5558	12.4875	-6.2908	10.4546	-0.0121
5	25.1131	5.0329	4.9898	14.8592	0.0124
				17.6239	-0.0105
Degrees of Freedom= 2				19.4262	0.0038
Confidence in First Term= 99.5%+					
Confidence in Last Term= 97.5%+					

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.2740	0.0071	38.6696	------	------
1	-0.9166	0.0647	-14.1625	0.1961	-0.0006
2	0.9705	0.1511	6.4231	0.1000	0.0017
3	-0.5324	0.1000	-5.3252	-0.0038	-0.0019
				-0.0919	0.0015
Degrees of Freedom= 1				-0.1559	-0.0006
Integral at x=1: 0.0061				------	------
Error in Integral: 0.0044					


Tetraethylsilane/Benzene
T = 50°C
o = observed
x = calculated
20
18
16
14
12
10
8
6
4
2
0
.2
.4
.6
.8
1.0
x21


Tetraethylsilane/Benzene
T = 50°C
o = observed
x = calculated
.4
.3
.2
.1
0
-.1
-.2
-.3
-.4
0
.2
.4
.6
.8
1.0
x_{21}

System: Ethylene Chloride/Benzene T= 20°C.

Reference: Sieg,Crutzen,Yost(1951):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
62.20	1.0000	1.0000	62.2000	1.0000	1.0000	------
64.40	0.8450	0.8140	52.4216	0.9974	1.0304	-0.0141
66.50	0.7030	0.6570	43.6905	0.9912	1.0240	-0.0107
68.60	0.5570	0.5080	34.8488	1.0059	1.0158	-0.0043
70.40	0.4060	0.3640	25.6256	1.0147	1.0050	0.0042
72.60	0.2230	0.2960	21.4896	1.5493	0.8771	0.2471
75.00	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

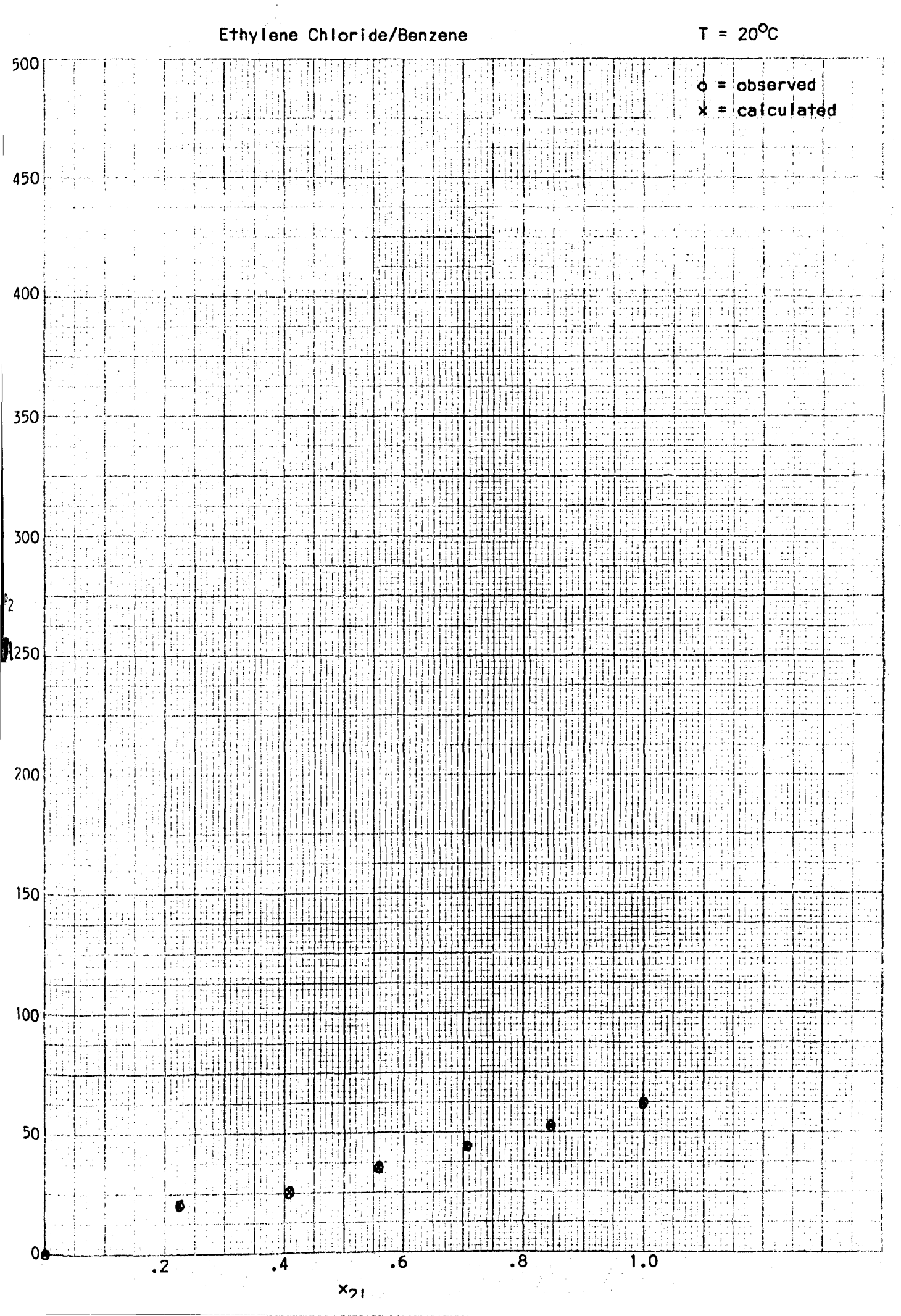
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	374.3391	2.0364	183.8257	62.2000	0.0000
2	-2443.6870	20.9355	-116.7244	52.4216	0.0000
3	7483.7832	78.9726	94.7643	43.6905	0.0000
4	-11192.5137	139.1470	-80.4366	34.8488	0.0000
5	8174.5363	115.9482	70.5016	25.6256	0.0000
6	-2334.2578	36.8781	-63.2965	21.4896	0.0000
				0.0000	0.0000

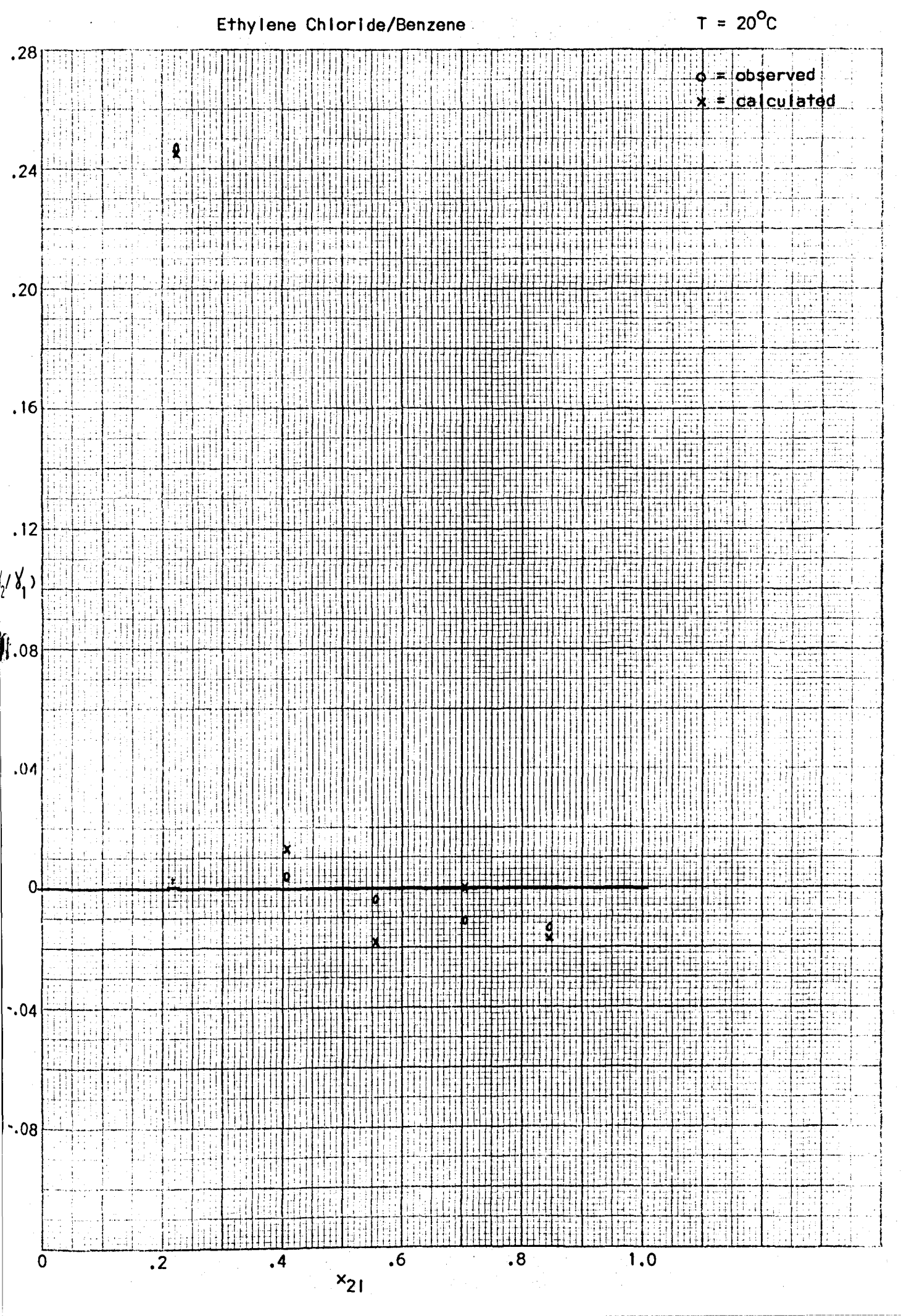
Degrees of Freedom= 1
Confidence in First Term= 99.5%+
Confidence in Last Term= 99.5%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	1.0399	0.1595	6.5200	------	------
1	-5.2159	1.0993	-4.7447	-0.0168	0.0027
2	8.3914	2.2395	3.7470	-0.0005	-0.0101
3	-4.3770	1.3917	-3.1450	-0.0184	0.0141
				0.0125	-0.0083
				0.2455	0.0016
				------	------

Degrees of Freedom= 1
Integral at x=1: 0.1348
Error in Integral: 0.0087


Ethylene Chloride/Benzene
T = 20°C
o = observed
x = calculated
500
450
400
350
300
250
200
150
100
50
0
.2
.4
.6
.8
1.0
x_{21}


Ethylene Chloride/Benzene
T = 20°C
o = observed
x = calculated
.28
.24
.20
.16
.12
.08
.04
0
-.04
-.08
0
.2
.4
.6
.8
1.0
x21

System: Ethylene Chloride/Benzene T= 45°C.

Reference: Sieg,Crutzen,Yost(1951):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
191.50	1.0000	1.0000	191.5000	1.0000	1.0000	------
198.20	0.8450	0.8210	162.7222	1.0056	1.0255	-0.0085
203.00	0.7030	0.6680	135.6708	1.0078	1.0172	-0.0040
207.80	0.5570	0.5200	108.0560	1.0130	1.0088	0.0018
211.80	0.4060	0.3730	79.0014	1.0161	1.0016	0.0062
217.00	0.2230	0.2040	44.2680	1.0366	0.9960	0.0174
223.20	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

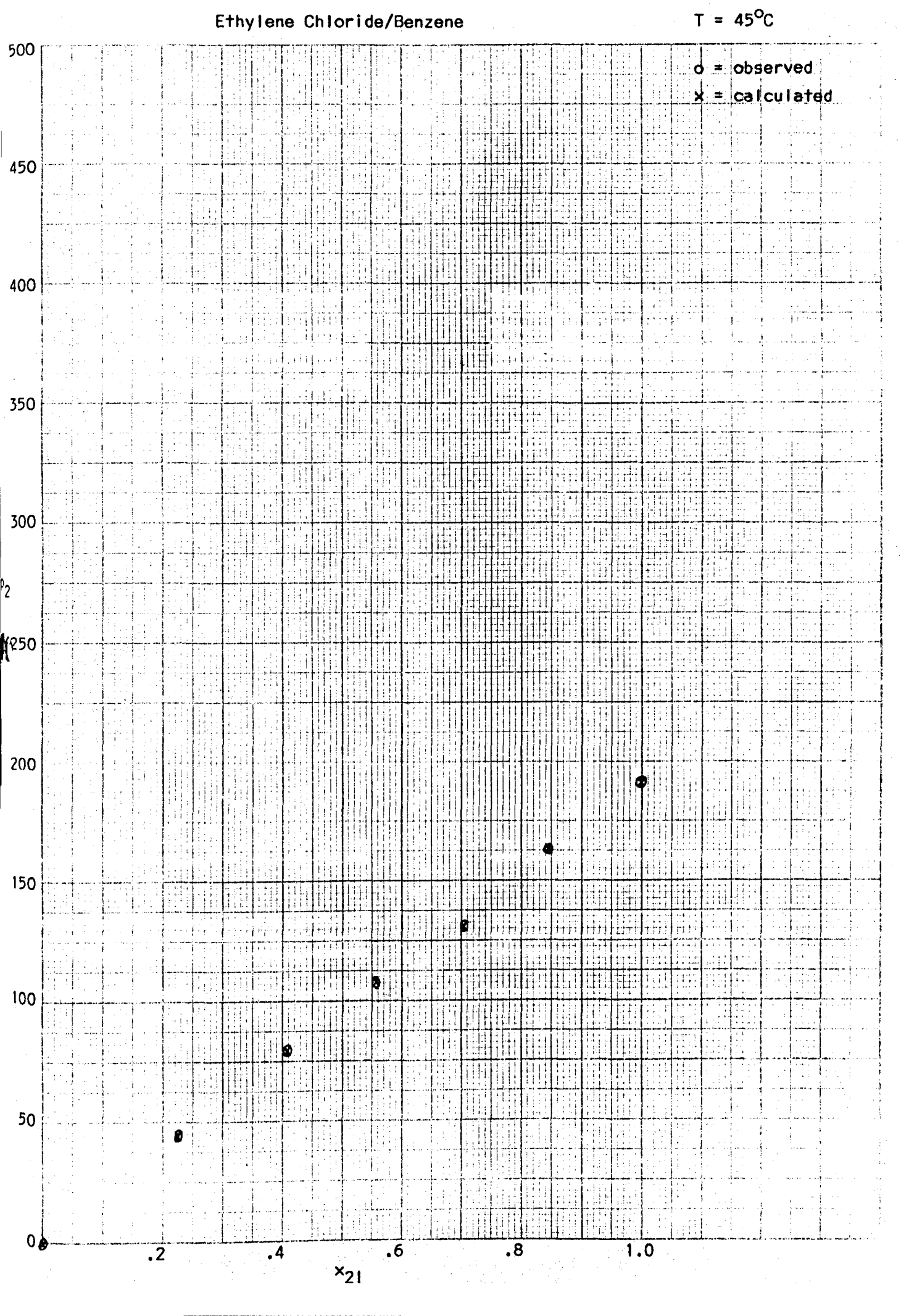
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	244.1669	6.2885	38.8273	191.5000	0.0000
2	-434.6848	64.6509	-6.7236	162.7222	0.0000
3	1497.2576	243.8748	6.1395	135.6708	0.0000
4	-2511.1180	429.6990	-5.8439	108.0560	0.0000
5	2029.3057	358.0590	5.6675	79.0014	0.0000
6	-633.4274	113.8831	-5.5621	44.2680	0.0000
				0.0000	0.0000

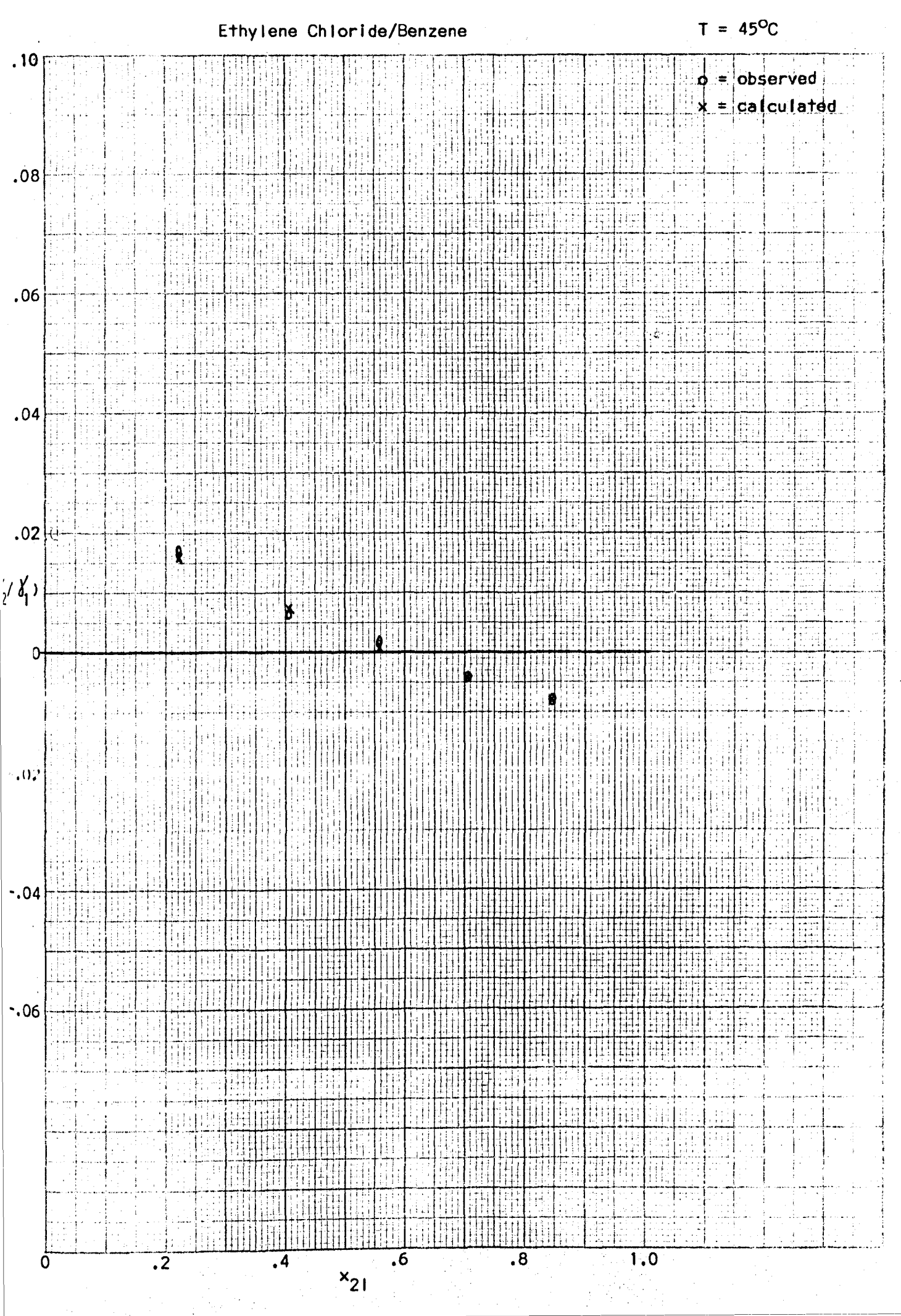
Degrees of Freedom= 1
Confidence in First Term= 99.0%+
Confidence in Last Term= 90.0%+

THERMODYNAMIC CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.0308	0.0033	9.4379	------	------
1	-0.0680	0.0135	-5.0182	-0.0082	-0.0003
2	0.0257	0.0125	2.0575	-0.0042	0.0002
				0.0009	0.0009
				0.0075	-0.0012
				0.0160	0.0004
				------	------

Degrees of Freedom= 2
Integral at x=1: 0.0054
Error in Integral: 0.0007


Ethylene Chloride/Benzene
T = 45°C
o = observed
x = calculated
500
450
400
350
300
250
200
150
100
50
0
.2
.4
.6
.8
1.0
x21


Ethylene Chloride/Benzene
T = 45°C
o = observed
x = calculated
.10
.08
.06
.04
.02
0
-.04
-.06
0
.2
.4
.6
.8
1.0
x_{21}

System: Ethylene Chloride/Benzene T= 70°C.

Reference: Sieg,Crutzen,Yost(1951):Physico-Chemical Constants of Binary Systems,Timmerman

P_{12}	x_{21}	x_{2v}	P_2	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
488.80	1.0000	1.0000	488.8000	1.0000	1.0000	------
499.90	0.8450	0.8250	412.4175	0.9985	1.0258	-0.0117
509.30	0.7030	0.6770	344.7961	1.0034	1.0067	-0.0014
518.40	0.5570	0.5270	273.1968	1.0034	1.0060	-0.0011
527.60	0.4060	0.3790	199.9604	1.0076	1.0025	0.0022
538.00	0.2230	0.2070	111.3660	1.0217	0.9980	0.0102
550.20	0.0000	0.0000	0.0000	1.0000	1.0000	------

PARTIAL PRESSURE CURVE FITTING:

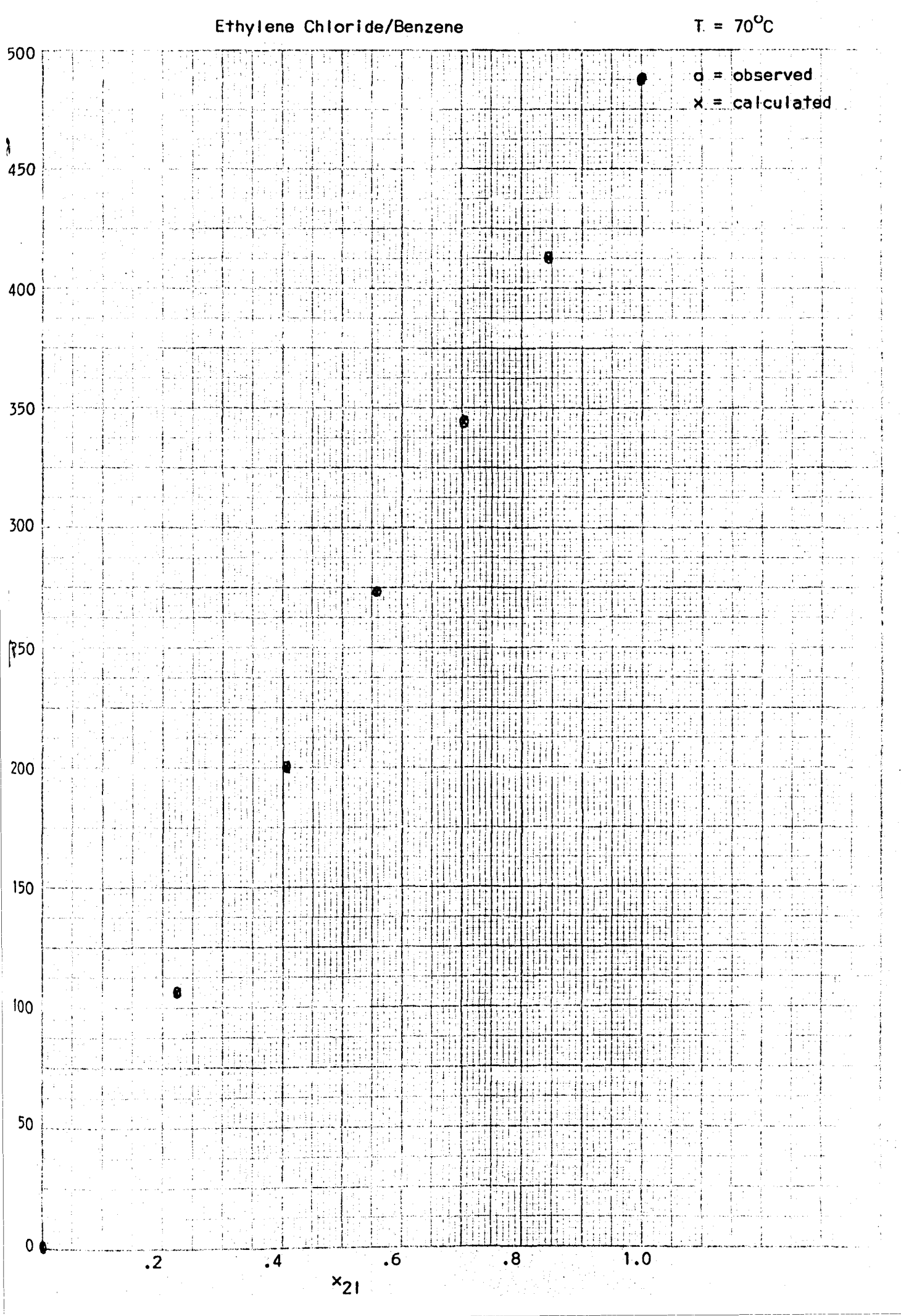
n	a_n	STD.ERROR	t	P_2 CALC.	DIF.
1	542.5600	15.3366	35.3768	488.7803	0.0197
2	-334.3734	118.3436	-2.8254	412.5444	-0.1269
3	813.1716	314.1870	2.5882	344.4953	0.3008
4	-865.0176	345.3790	-2.5045	273.5516	-0.3548
5	332.4398	134.3668	2.4741	199.7468	0.2136
				111.4247	-0.0587
				0.0000	0.0000

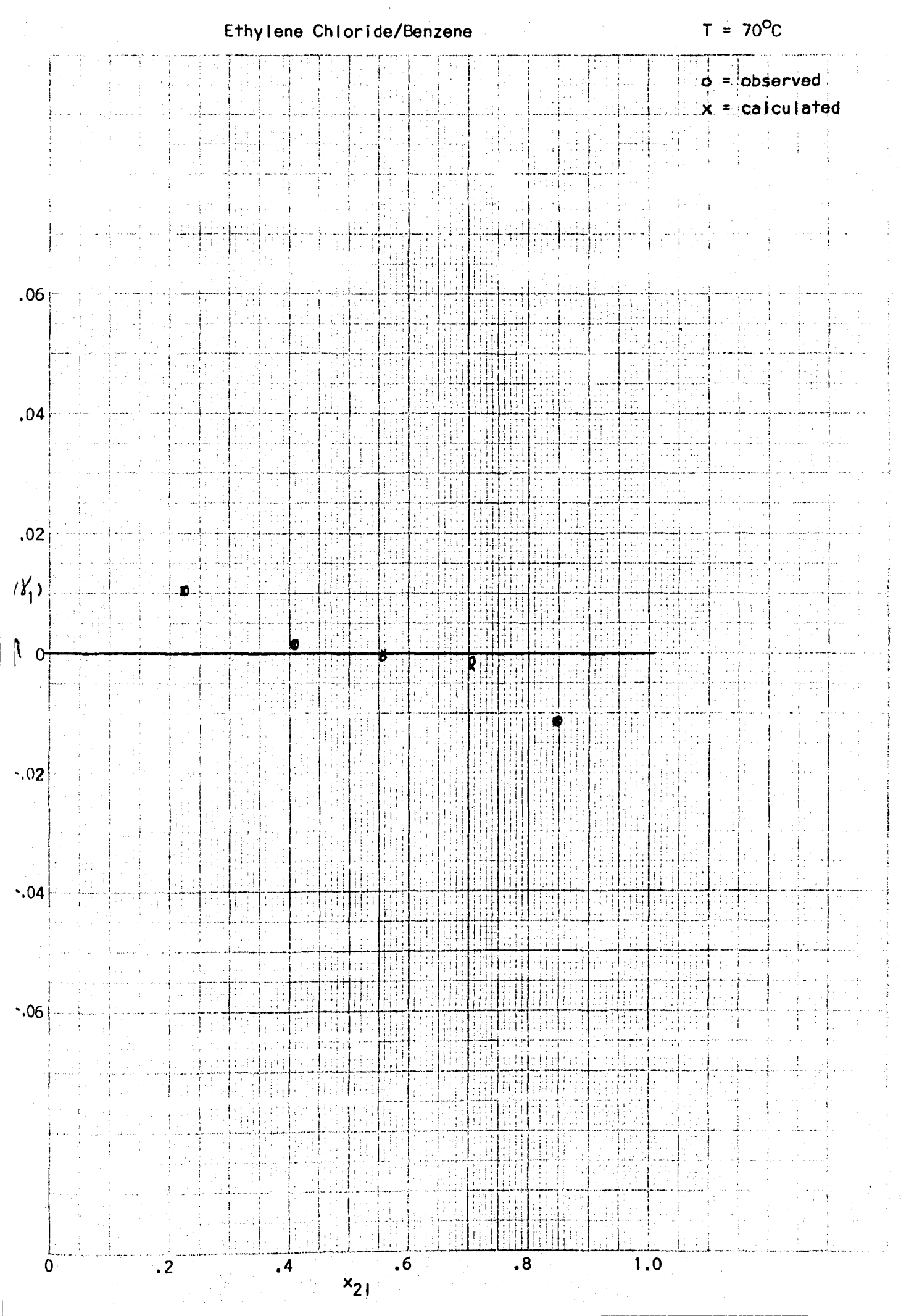
Degrees of Freedom= 2
Confidence in First Term= 99.5%+
Confidence in Last Term= 90.0%+

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.0477	0.0144	3.3116	------	------
1	-0.2605	0.0990	-2.6324	-0.0115	-0.0002
2	0.4869	0.2016	2.4153	-0.0023	0.0009
3	-0.3094	0.1253	-2.4697	0.0002	-0.0013
				0.0015	0.0007
				0.0104	-0.0001
				------	------

Degrees of Freedom= 1
Integral at x=1: 0.0024
Error in Integral: 0.0008


Ethylene Chloride/Benzene
T = 70°C
o = observed
x = calculated
500
450
400
350
300
250
200
150
100
50
0
.2
.4
.6
.8
1.0
x21


Ethylene Chloride/Benzene
T = 70°C
o = observed
x = calculated
.06
.04
.02
(γ1)
0
-.02
-.04
-.06
0
.2
.4
.6
.8
1.0
x21

THERMODYNAMIC CONSISTENCY TEST DATA

System: Isopropyl Alcohol/Benzene T= 45°C.

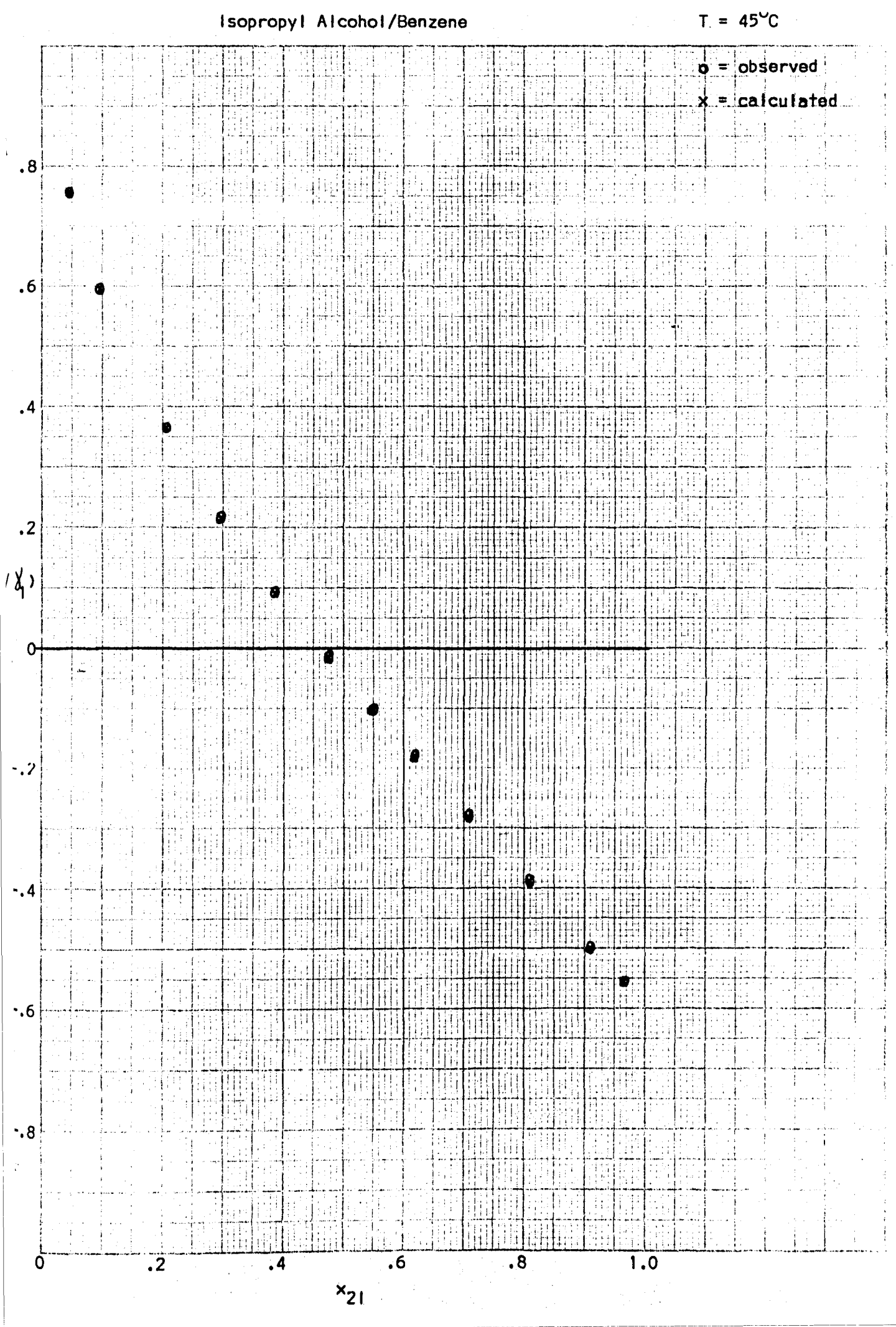
Reference: Jaques,J.Chem.Ed. 42,12,651(1965)

p_2^o=136.05 p_1^o=223.66

P_{12}	x_{21}	x_{2v}	γ_2	γ_1	$\log(\gamma_2/\gamma_1)$
252.50	0.0472	0.1467	5.7683	1.0111	0.7563
264.13	0.0980	0.2066	4.0928	1.0388	0.5955
272.06	0.2047	0.2663	2.6015	1.1222	0.3652
273.40	0.2960	0.2953	2.0048	1.2236	0.2144
272.22	0.3862	0.3211	1.6636	1.3462	0.0919
269.49	0.4753	0.3463	1.4432	1.5011	-0.0171
264.92	0.5504	0.3692	1.3062	1.6618	-0.1046
259.35	0.6198	0.3951	1.2152	1.8449	-0.1813
247.70	0.7096	0.4378	1.1233	2.1440	-0.2807
227.14	0.8073	0.5107	1.0562	2.5787	-0.3877
189.28	0.9120	0.6658	1.0157	3.2140	-0.5003
159.80	0.9655	0.8252	1.0039	3.6200	-0.5570

THERMODYNAMIC CONSISTENCY CURVE FITTING:

n	a_n	STD. ERROR	t	$\log(\gamma_2/\gamma_1)$ CALC.	DIF.
0	0.9693	--------	-------	0.7562	-0.0001
1	-5.4648	0.2699	-20.2443	0.5957	0.0002
2	24.0553	3.4531	6.9664	0.3645	-0.0006
3	-93.6490	21.3445	-4.3875	0.2155	0.0010
4	242.5958	72.3163	3.3547	0.0912	-0.0007
5	-396.0445	141.2832	-2.8032	-0.0175	-0.0004
6	388.3149	158.5514	2.4491	-0.1036	0.0009
7	-208.3053	94.8360	-2.1965	-0.1816	-0.0003
8	46.9382	23.4099	2.0051	-0.2811	-0.0004
				-0.3873	0.0003
Degrees of Freedom= 8				-0.5004	-0.0002
Integral at x=1: 0.0066				-0.5570	0.0000
Error in Integral: 0.0005					


Isopropyl Alcohol/Benzene
T = 45°C
o = observed
x = calculated
.8
.6
.4
.2
(γ1)
0
-.2
-.4
-.6
-.8
0
.2
.4
.6
.8
1.0
x21

Appendix 2

Programs

```
)LOAD HARRY
SAVED  20.11.11 09/08/70
      ∇CONVERT[□]∇
    ∇ CONVERT
[1]   'INPUT MOLE FRACTION SOLUTE IN LIQUID'
[2]   CSUL←□
[3]   'INPUT MOLE FRACTION SOLUTE IN VAPOR'
[4]   CSUV←□
[5]   'INPUT TOTAL PRESSURE'
[6]   PT←□
[7]   CSVV←1-CSUV
[8]   CSVL←1-CSUL
[9]   PPSU←PT×CSUV
[10]  PPSV←PT×CSVV
[11]  Z←PT AND CSUL AND CSUV AND CSVL AND CSVV AND PPSU AND PPSV
[12]  ''
[13]  '   PT         CSUL       CSUV       CSVL      CSVV       PPSU        PPSV'
[14]  ''
[15]  8 2 10 4 10 4 10 4 10 4 12 4 12 4 DFT Z
[16]  ''
    ∇


      ∇THERMO[□]∇
    ∇ THERMO
[1]   'INPUT PRESSURE PURE SOLUTE'
[2]   POSU←□
[3]   'INPUT PRESSURE PURE SOLVENT'
[4]   POSV←□
[5]   GSU←((CSUV×PT)÷CSUL)÷POSU
[6]   GSV←((CSVV×PT)÷CSVL)÷POSV
[7]   LOG←(●(GSU÷GSV))÷2.303
[8]   ZZ←GSU AND GSV AND LOG
[9]   ''
[10]  '      GSU      GSV      LOG(GSU/GSV)'
[11]  ''
[12]  10 4 10 4 10 4 DFT ZZ
[13]  ''
    ∇
```

```
)LOAD FITTING
SAVED  10.53.17 08/08/70
      ∇HARRYFIT[⎕]∇
    ∇ HARRYFIT
[1]   'INPUT MOLE FRACTION OF SOLUTE IN LIQUID, X'
[2]   X←⎕
[3]   'INPUT PARTIAL PRESSURE OF SOLUTE, Y'
[4]   Y←⎕
[5]   'INPUT ORDER OF EQUATION, M'
[6]   M←⎕
[7]   MATY←((⍴Y),1)⍴Y
[8]   KOUNTER←1
[9]   X2←0⍴1
[10] CYCLE1:X1←X*(KOUNTER)
[11]  X2←X2,X1
[12]  KOUNTER←KOUNTER+1
[13]  →(KOUNTER≤M)/CYCLE1
[14]  MATX←⍉((M,(⍴X))⍴X2)
[15]  CINV←⌹((⍉MATX)+.×(MATX))
[16]  MATB←(((CINV)+.×(⍉MATX))+.×(MATY))
[17]  S2←(((⍉MATY)+.×(MATY))-(((⍉MATB)+.×(⍉MATX))+.×MATY))÷((⍴X)-M)
[18]  KOUNTER←1
[19]  VARB←0⍴1
[20] CYCLE2:VB←S2×(CINV[KOUNTER;KOUNTER])
[21]  VARB←VARB,,VB
[22]  KOUNTER←KOUNTER+1
[23]  →(KOUNTER≤M)/CYCLE2
[24]  MATB←M⍴MATB
[25]  TB←MATB÷(VARB*0.5)
[26]  KOUNTER←1
[27]  X3←0⍴1
[28] CYCLE3:X4←KOUNTER
[29]  X3←X3,X4
[30]  KOUNTER←KOUNTER+1
[31]  →(KOUNTER≤M)/CYCLE3
[32]  ''
[33]  ''
[34]  'RESULTS'
[35]  Z←X3 AND MATB AND(VARB*0.5) AND TB
[36]  '       TERM          COEFF.        STD.ERROR        T VALUE'
[37]  ''
[38]  15 4 15 4 15 4 15 4 DFT Z
[39]  ''
[40]  'DEGREES OF FREEDOM:';(⍴X)-M
[41]  ''
[42]  'PLOT?'
[43]  HEB←⎕
[44]  →(HEB>1)/0
[45]  KOUNTER←1
[46]  YC←0⍴1
[47] CYCLE4:YCC←(MATB[KOUNTER])×(X*KOUNTER)
[48]  YC←YC,YCC
[49]  KOUNTER←KOUNTER+1+
```

```
[50]  →(KOUNTER≤M)/CYCLE4
[51]  YC←+⌿((M,(⍴X))⍴YC)
[52]  DF←Y-YC
[53]  ''
[54]  'LENGTH IN INCHES TIMES 10'
[55]  LV←⍬
[56]  'WIDTH IN INCHES TIMES 10'
[57]  LH←⍬
[58]  ''
[59]  (LV,LH) PLOT Y AND YC VS X
[60]  ''
[61]  '(o) OBSERVED        (*) FITTED'
[62]  ''
[63]  ''
[64]  ZZ←X AND Y AND YC AND DF
[65]  '      X            Y       Y CALC.        DIF.'
[66]  ''
[67]  10 4 10 4 10 4 10 4 DFT ZZ
      ∇
```

```
)LOAD THERMOFIT
SAVED  17.15.00 08/26/70
      ∇HARRYFIT[□]∇
    ∇ HARRYFIT
[1]    'INPUT MOLE FRACTION OF SOLUTE IN LIQUID, X'
[2]    X←□
[3]    'INPUT LOG GSU/GSV, Y'
[4]    Y←□
[5]    'INPUT ORDER OF EQUATION, M'
[6]    M←□
[7]    MATY←((ρY),1)ρY
[8]    KOUNTER←0
[9]    X2←0ρ1
[10] CYCLE1:X1←X*(KOUNTER)
[11]   X2←X2,X1
[12]   KOUNTER←KOUNTER+1
[13]   →(KOUNTER≤M)/CYCLE1
[14]   MATX←⌹(((M+1),(ρX))ρX2)
[15]   CINV←INV((⌹MATX)+.×(MATX))
[16]   MATB←(((CINV)+.×(⌹MATX))+.×(MATY))
[17]   S2←(((⌹MATY)+.×(MATY))-(((⌹MATB)+.×(⌹MATX))+.×MATY))÷((ρX)-(M+1∇))
[18]   KOUNTER←1
[19]   VARB←0ρ1
[20] CYCLE2:VB←S2×(CINV[KOUNTER;KOUNTER])
[21]   VARB←VARB,,VB
[22]   KOUNTER←KOUNTER+1+
[23]   →(KOUNTER≤(M+1))/CYCLE2
[24]   MATB←(M+1)ρMATB
[25]   TB←MATB÷(VARB*0.5)
[26]   KOUNTER←0
[27]   X3←0ρ1
[28] CYCLE3:X4←KOUNTER
[29]   X3←X3,X4
[30]   KOUNTER←KOUNTER+1
[31]   →(KOUNTER≤M)/CYCLE3
[32]   X5←0ρ1
[33]   KOUNTER←1
[34] CYCLE5:X6←KOUNTER
[35]   X5←X5,X6
[36]   KOUNTER←KOUNTER+1
[37]   →(KOUNTER≤(M+1))/CYCLE5
[38]   ITGL←+/(MATB÷X5)
[39]   EROR←+/((((VARB*0.5)*2)÷(X5*2))*0.5)
[40]   ''
[41]   ''
[42]   'RESULTS'
[43]   Z←X3 AND MATB AND∇(VARB*0.5) AND TB
```

```
[44]   '        TERM            COEFF.          STD.ERROR        T VALUE'
[45]   ''
[46]   15 4+15 4 15 4 15 4 DFT Z
[47]   ''
[48]   'DEGREES OF FREEDOM:';(ρX)-(M+1)
[49]   'INTEGRAL AT X=1: ';ITGL
[50]   'ERROR IN INTEGRAL: ';EROR
[51]   ''
[52]   'PLOT?'
[53]   HEB←⍞
[54]   →(HEB>1)/0
[55]   KOUNTER←1
[56]   YC←0ρ1
[57]  CYCLE4:YCC←(MATB[KOUNTER])×(X*(KOUNTER-1))
[58]   YC←YC,YCC
[59]   KOUNTER←KOUNTER+1
[60]   →(KOUNTER≤(M+1))/CYCLE4
[61]   YC←+⌿(((M+1),(ρX))ρYC)
[62]   DF←Y-YC
[63]   ''
[64]   'LENGTH IN INCHES TIMES 10'
[65]   LV←⍞
[66]   'WIDTH IN INCHES TIMES 10'
[67]   LH←⍞
[68]   ''
[69]   (-1,LH) PLOT Y AND YC VS X
[70]   ''
[71]   '(o) OBSERVED        (*) FITTED'
[72]   ''
[73]   ''
[74]   ZZ←X AND Y AND YC AND DF
[75]   '      X              Y        Y CALC.          DIF.'
[76]   ''
[77]   10 4 10 4 10 4 10 4 DFT ZZ
       ∇
```

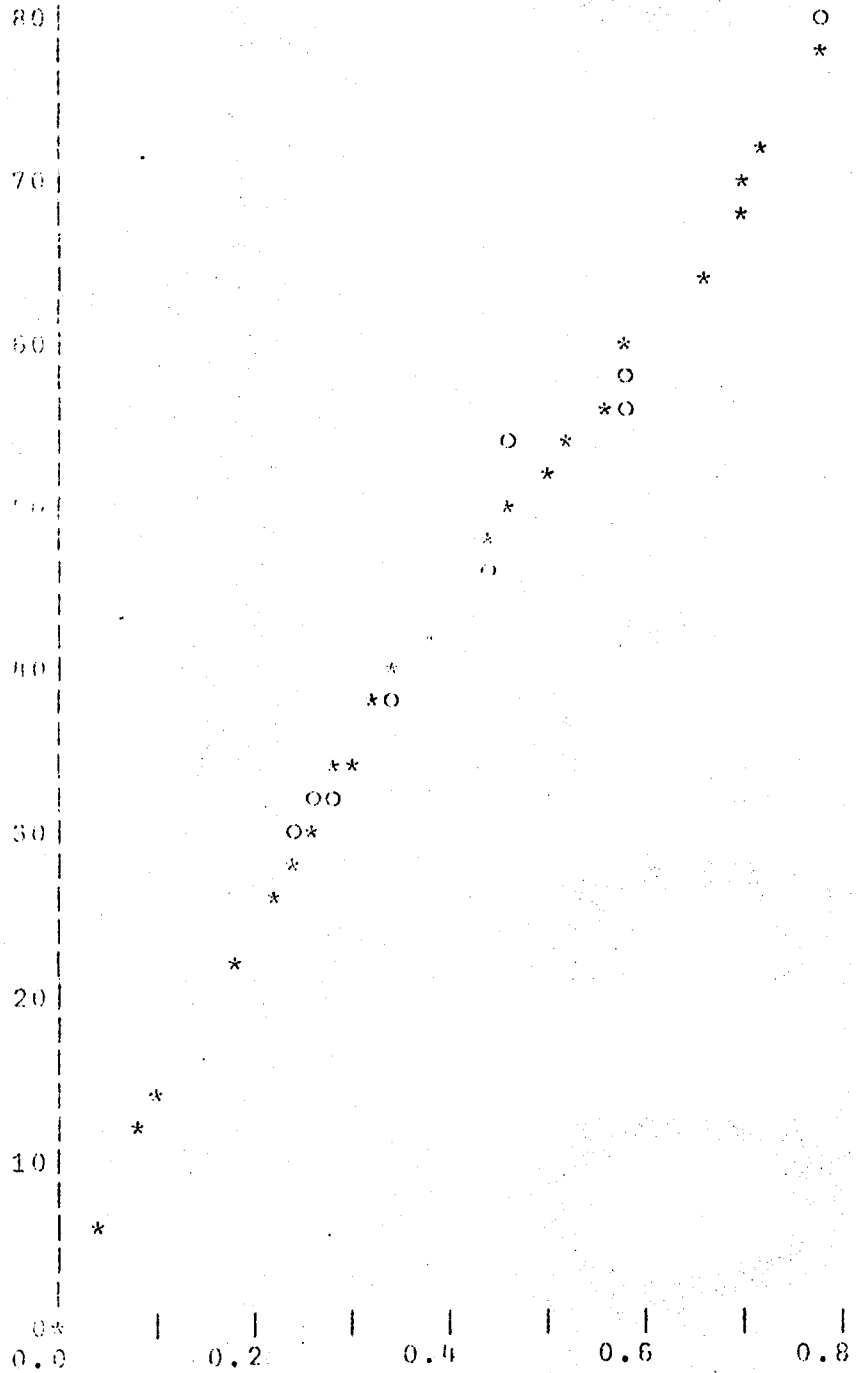
```
        HARRYFIT
INPUT MOLE FRACTION OF SOLUTE IN LIQUID, X
[]:
        CSUL
INPUT PARTIAL PRESSURE OF SOLUTE, Y
[]:
        PPSU
INPUT ORDER OF EQUATION, M
[]:
        3
```

1.0000	150.5611	5.2950	25.4455
2.0000	123.[illegible]	22.3715	[illegible]
3.0000	100.2567	21.1887	8.7320

DEGREES OF FREEDOM:24

PLOT?
1:
YES

LENGTH IN INCHES TIMES 10
1:
40
WIDTH IN INCHES TIMES 10
1:
50



(*) OBSERVED (*) FITTED

X	Y	Y CALC.	DIF.
.0000	.0000	.0000	.0000
.0459	6.3520	6.6170	-.2649
.0848	11.3986	11.7936	-.3950
.1060	13.9507	14.4618	-.5111
.1750	21.9685	22.4790	-.5105
.2110	28.3304	28.3947	-.0257
.2337	29.8604	28.6082	1.2513
.2528	31.1885	30.9873	.7012
.2850	32.9386	33.5455	-.6069
.2915	33.9228	34.1476	-.2248
.3270	37.2589	37.3564	-.0975
.3481	37.6272	39.2076	-1.5804
.3888	41.4137	42.6850	-1.2713
.4370	45.1580	46.6912	-1.5332
.4480	48.7925	47.5949	1.1976
.4450	46.7322	47.3487	-.6165
.4699	54.6890	49.3885	5.3005
.4958	51.3205	51.5071	-.1866
.5297	54.5713	54.2925	.2788
.5600	56.9330	56.8115	.1215
.5769	56.7944	58.2351	-1.4407
.5860+	58.7811	59.0085	-.2274
.6520	63.7554	64.8066	-1.0512
.6938	68.9236	69.7034	-.2202
.7049	69.2816	69.7745	-.4929
.7180	71.0927	71.0603	.0335
.7890	79.1415	78.4943	.6472

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AUTOBIOGRAPHY

Harold Edward Bennett was born on December 29, 1944 in Jersey City, New Jersey. He attended Jersey City public schools, entered Fairleigh Dickinson University, Rutherford, New Jersey in September, 1962, and received his Bachelor of Science Degree in Chemistry in June, 1966. During the summers of 1964 and 1965, he worked as a laboratory technician in toiletry development with Philip Morris in Hoboken, New Jersey. After graduation he joined Philip Morris as an assistant scientist in toiletries and medical product development. He started work on his Master of Science Degree at Stevens Institute of Technology in Hoboken, New Jersey and transferred to the University of Richmond when he moved to Richmond, Virginia with Philip Morris in September, 1967. He remained with Philip Morris until September, 1970 when he Joined Avon Products Co. as a product evaluator. He is a member of the American Chemical Society and the Society of Cosmetic Chemists.